

Supporting Information

for

Carbon dioxide hydrogenation to aromatic hydrocarbons by using an iron/iron oxide nanocatalyst

Hongwang Wang*¹, Jim Hodgson¹, Tej B. Shrestha², Prem S. Thapa³, David Moore³, Xiaorong Wu⁴,
Myles Ikenberry⁵, Deryl L. Troyer², Donghai Wang⁴, Keith L. Hohn⁵ and Stefan H. Bossmann*¹

Address: ¹Kansas State University, Department of Chemistry, 201CBC Building, Manhattan, KS 66506, USA, 001-785-532-6817; ²Kansas State University, Department of Anatomy & Physiology, 130 Coles Hall, Manhattan, KS 66506, USA; ³University of Kansas, Microscopy and Analytical Imaging Laboratory, 1043 Haworth, Lawrence, KS 66045, USA; ⁴Kansas State University, Department of Biological and Agricultural Engineering, 150 Seaton Hall, Manhattan, KS 66506, USA and ⁵Kansas State University, Department of Chemical Engineering, 1016 Durland Hall, Manhattan, KS 66506, USA

Email: Hongwang Wang* - hongwang@ksu.edu; Stefan H. Bossmann* - sbossmann@ksu.edu

*Corresponding author

Additional experimental data

Reaction kinetics

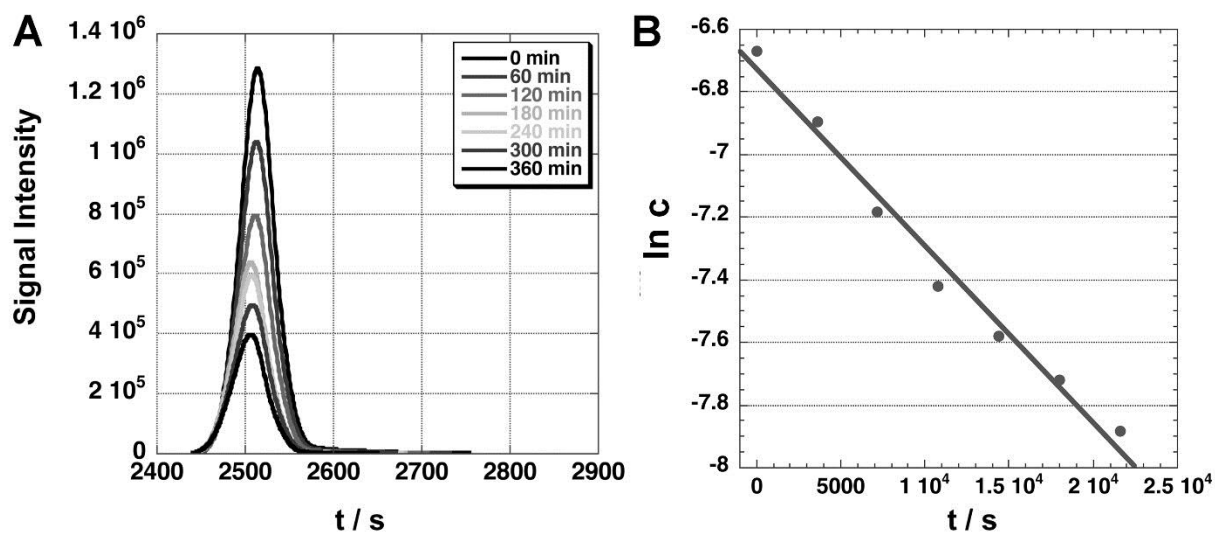


Figure S1: Consumption of CO₂ at 400 °C. A: CO₂ peak as a function of reaction time, as recorded by GC-MS. B: The reaction is a heterogeneous first order kinetics, as the plot $\ln(\text{signal intensity})$ vs t indicates.

Additional GC-MS chromatograms and mass spectra

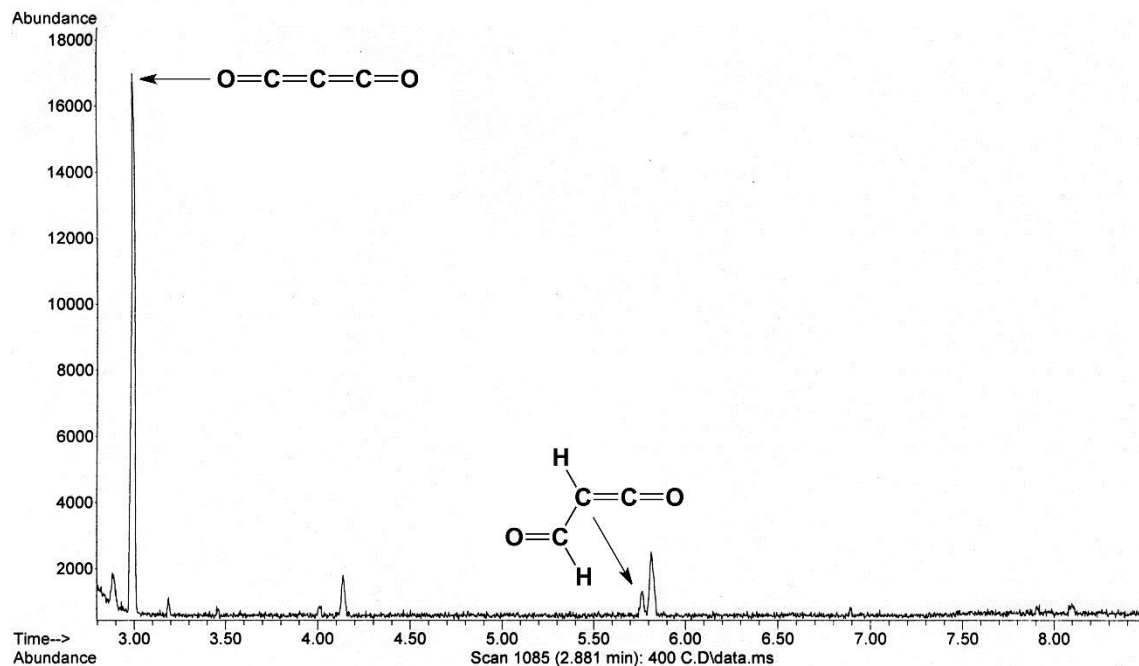


Figure S2: GC-MS chromatogram showing the major reaction intermediates that are formed at 400 °C.

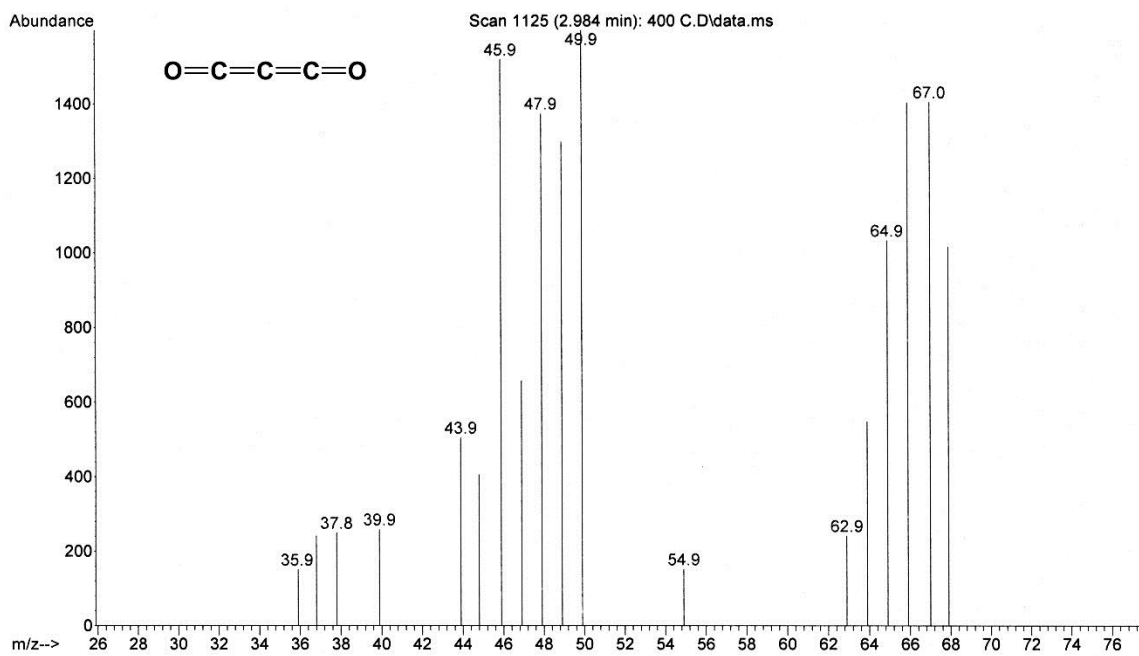


Figure S3: Mass spectrum of carbon suboxide (C_3O_2).

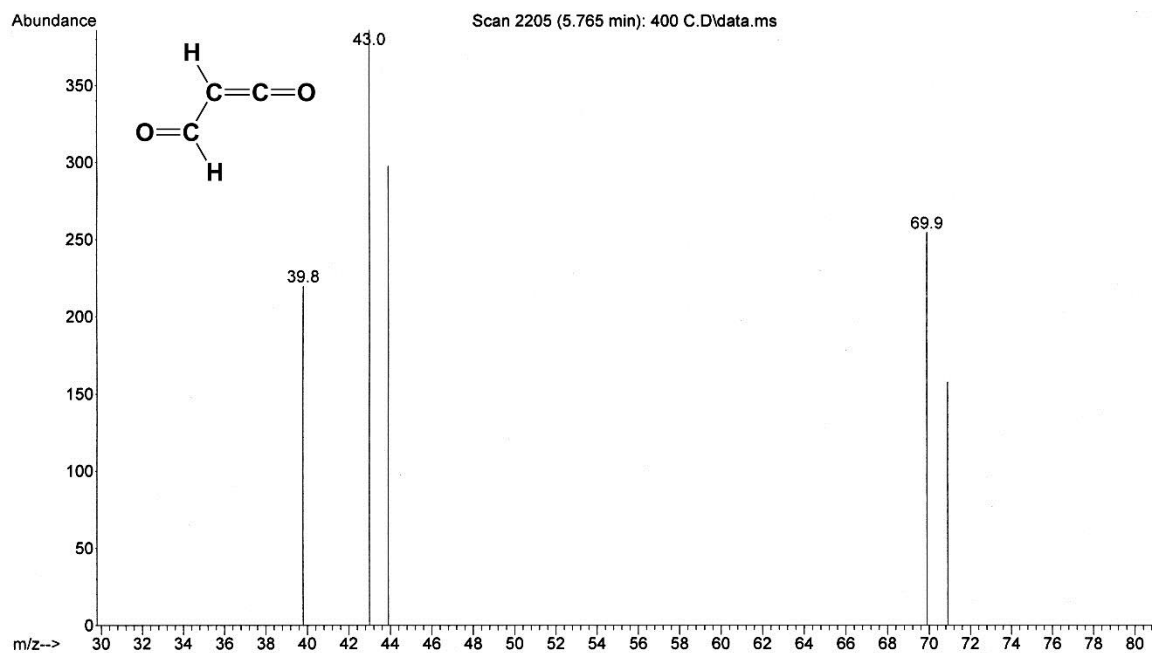


Figure S4: Mass spectrum of 3-oxoacrylaldehyde ($C_3H_2O_2$).

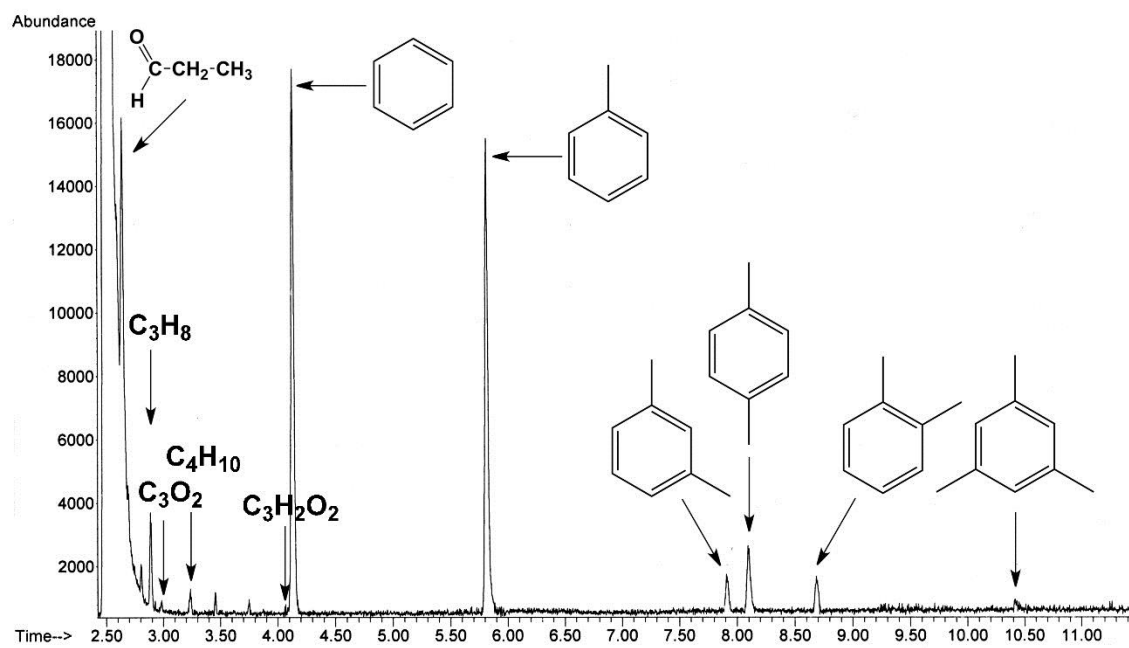


Figure S5: GC-MS chromatogram showing the major reaction products that are formed at 500 °C.

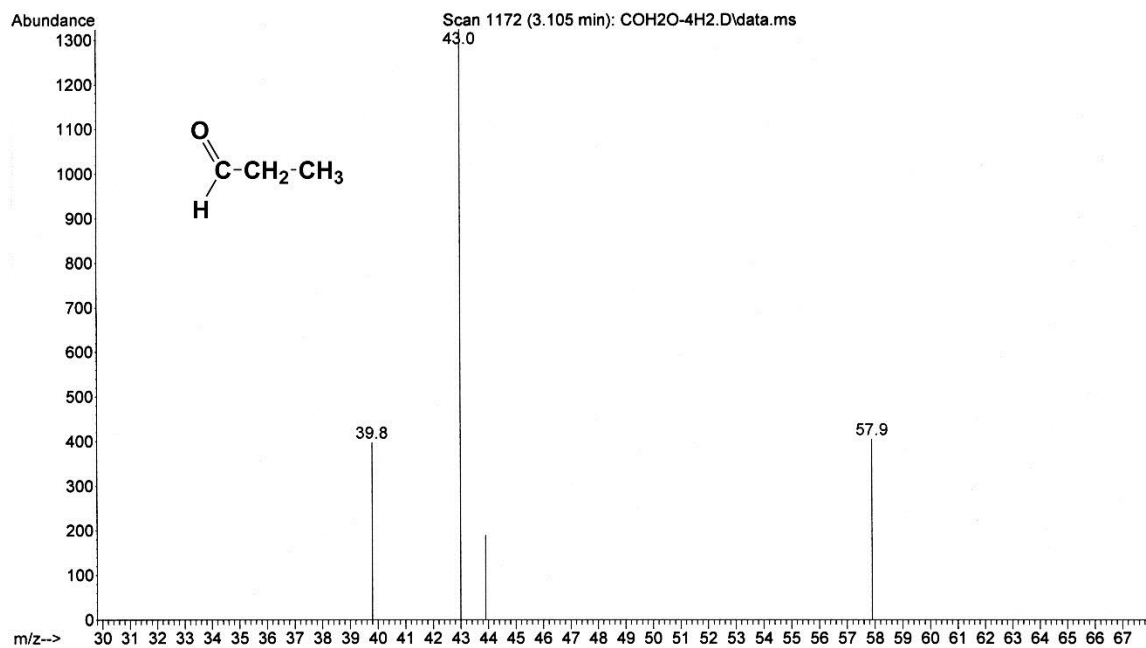


Figure S6: Mass spectrum of propionaldehyde (C_3H_6O).

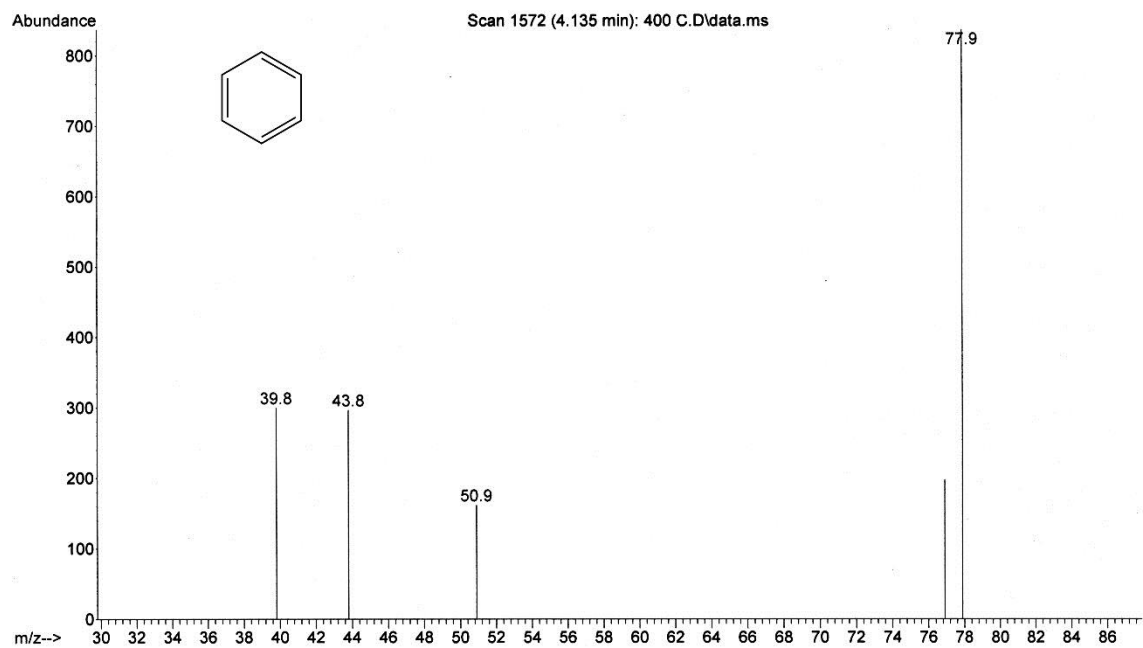


Figure S7: Mass spectrum of benzene (C_6H_6).

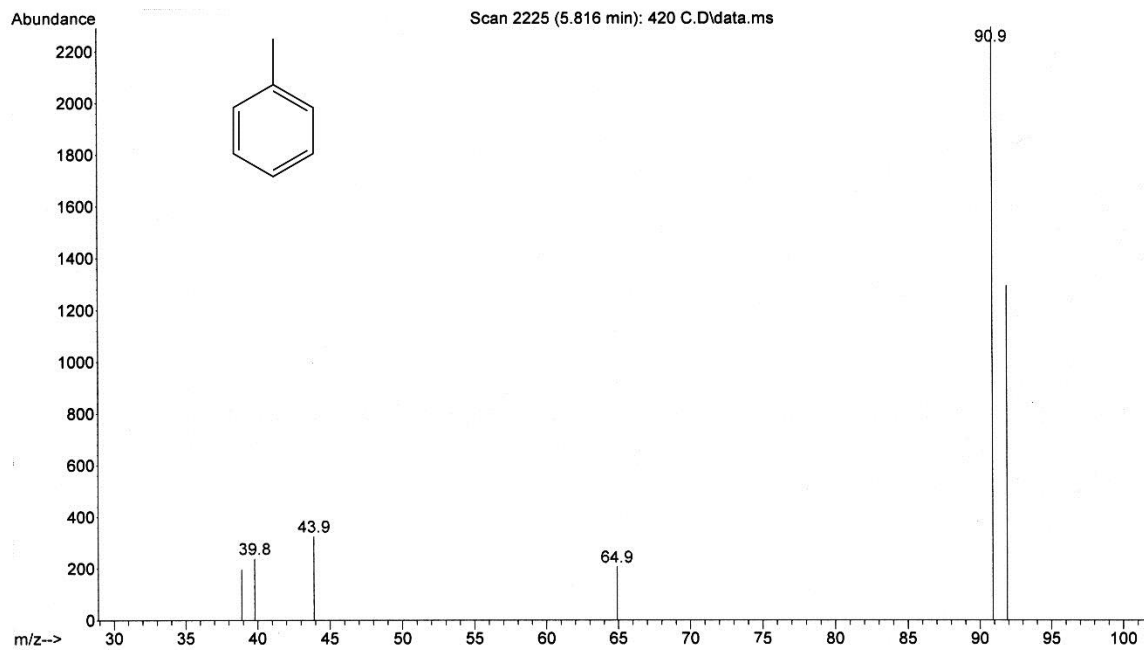


Figure S8: Mass spectrum of toluene (C_7H_8).

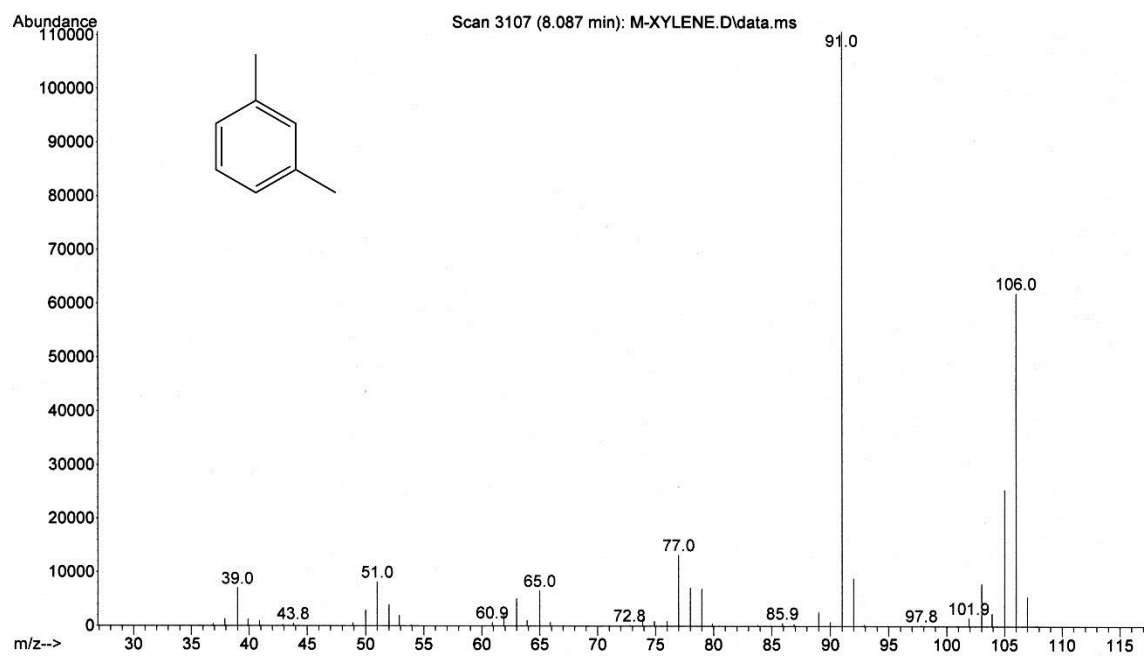


Figure S9: Mass spectrum of *meta*-xylene (C_8H_{10}).

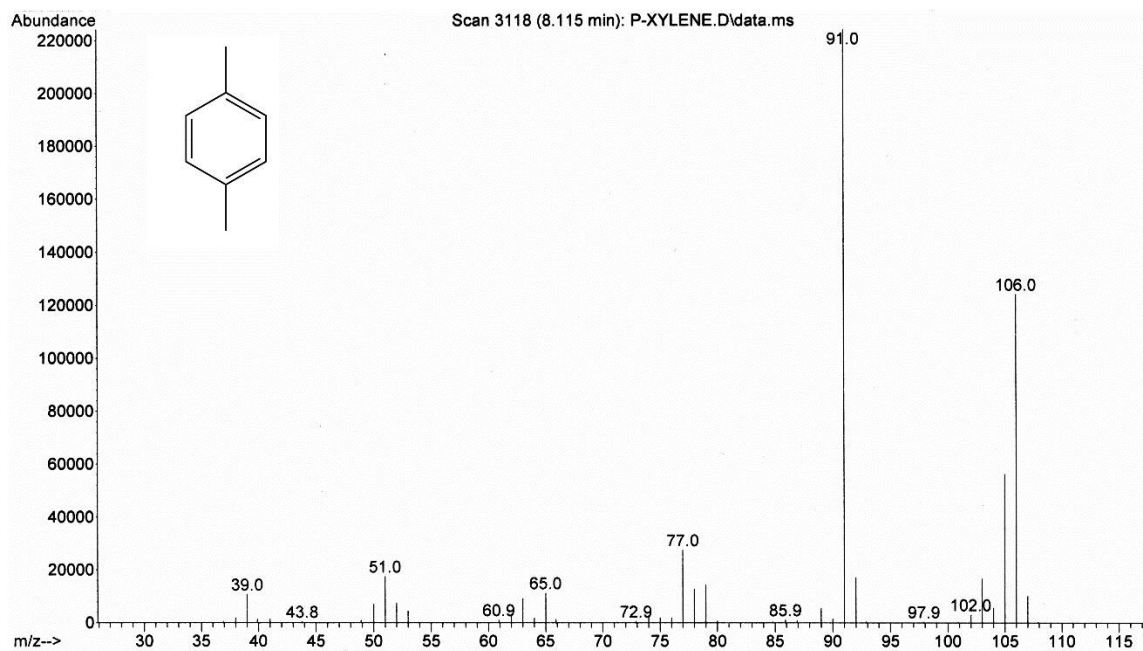


Figure S10: Mass spectrum of *para*-xylene (C_8H_{10}).

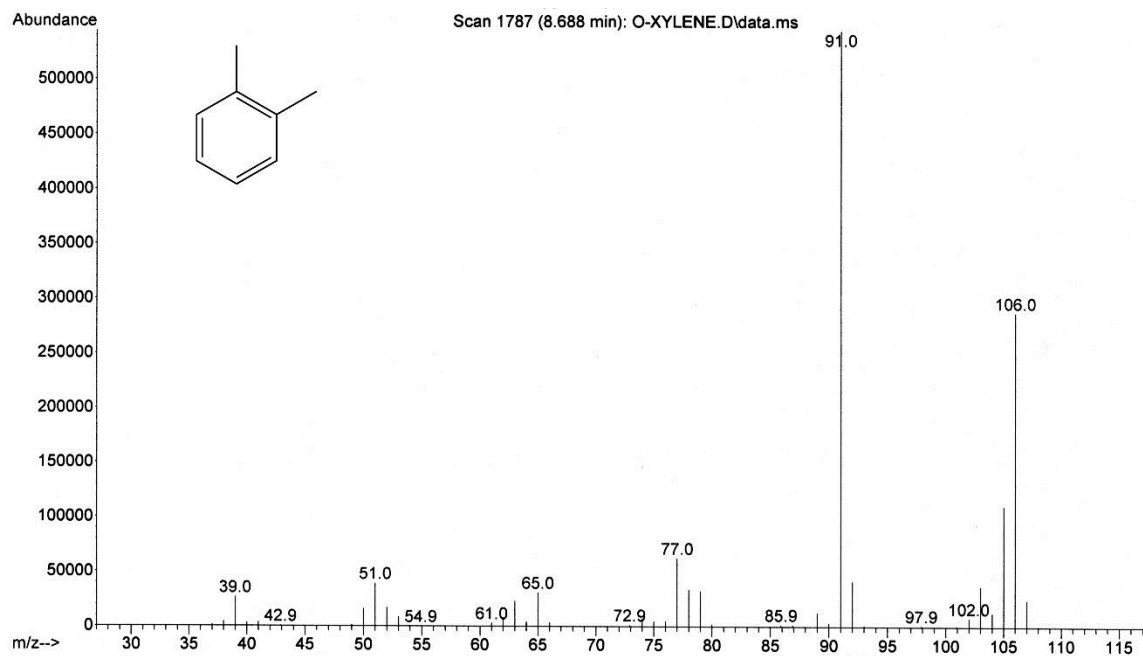


Figure S11: Mass spectrum of *ortho*-xylene (C_8H_{10}).

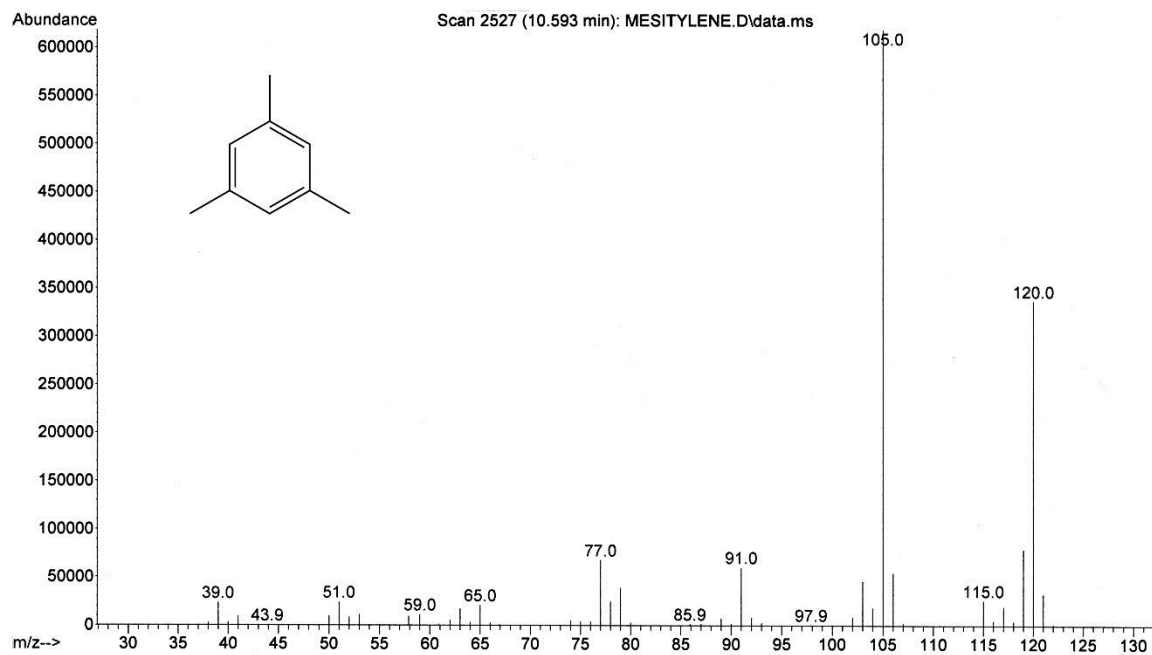


Figure S12: Mass spectrum of mesitylene (C_9H_{12}).

Additional XRD Spectra

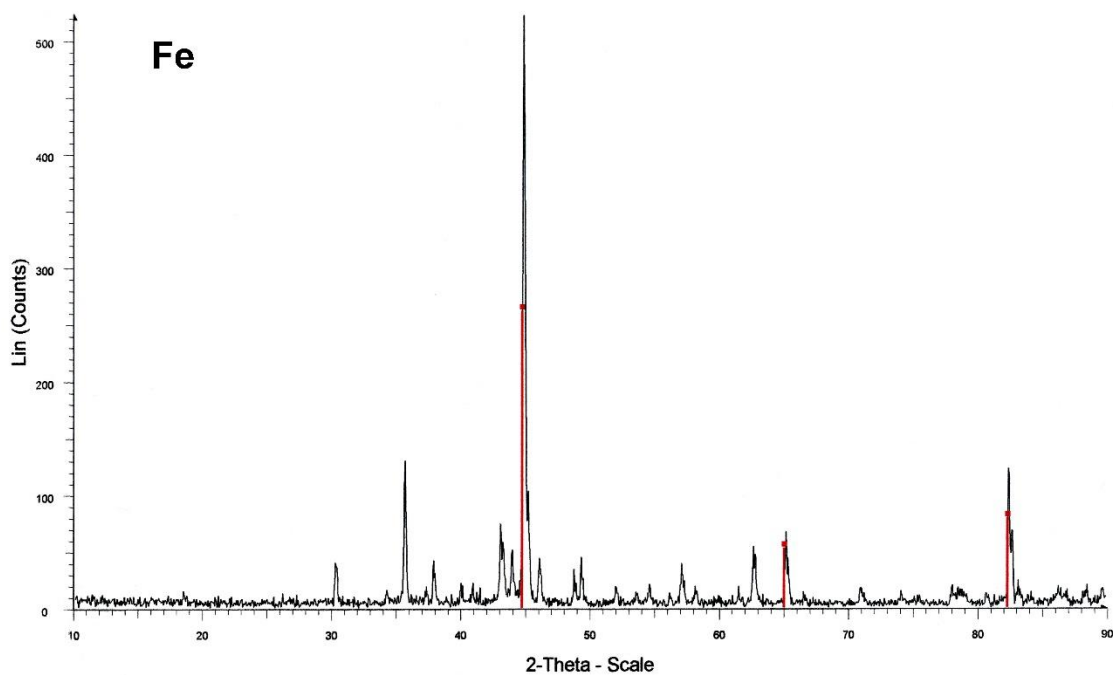


Figure S13: X-ray diffractogram of the Fe/Fe₃O₄-catalyst after 5 catalytic runs (2 h each).

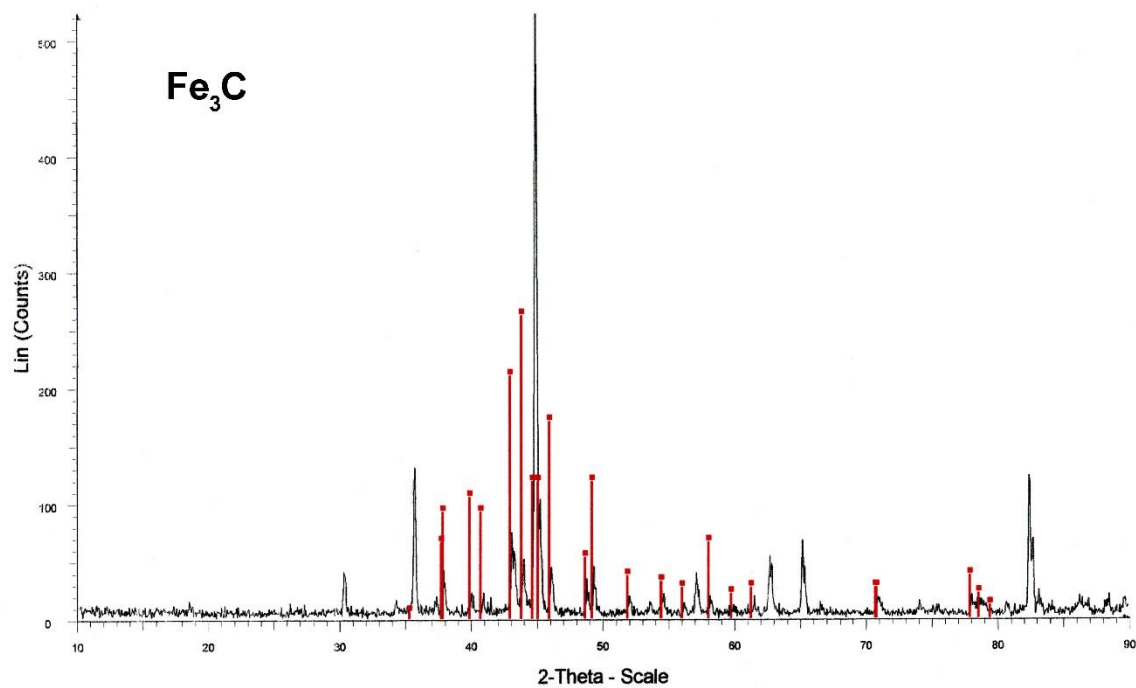


Figure S14: X-ray diffractogram of the Fe/Fe₃O₄-catalyst after 5 catalytic runs (2 h each).

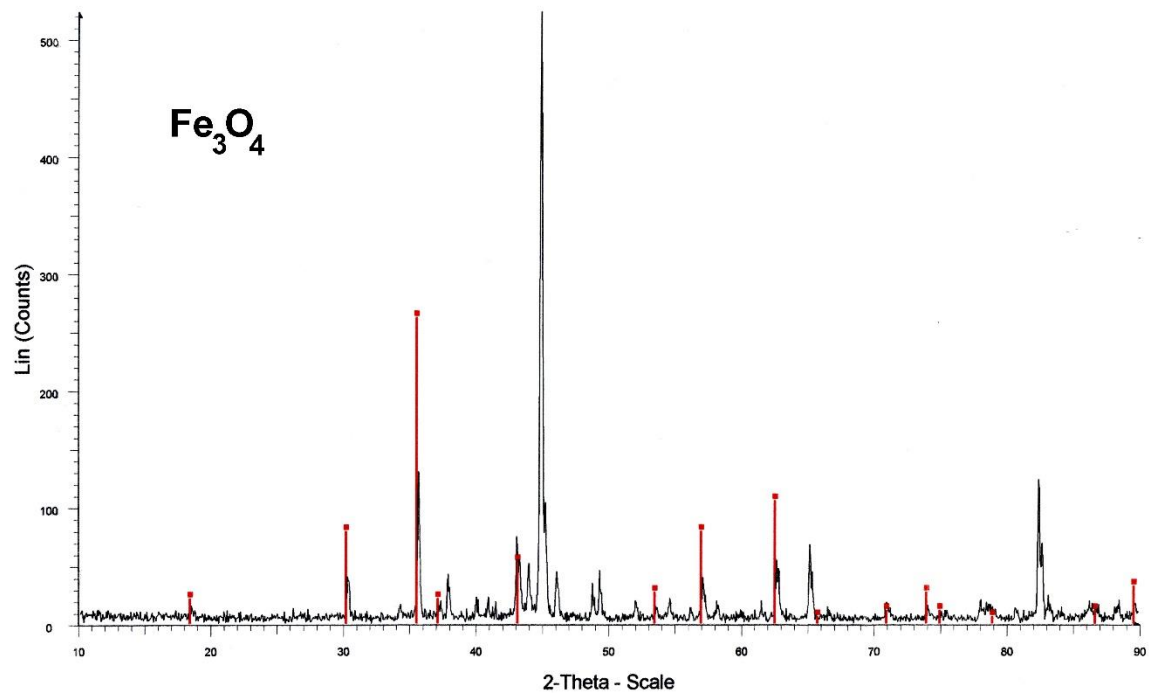


Figure S15: X-ray diffractogram of the Fe/Fe₃O₄-catalyst after 5 catalytic runs (2 h each).