

Supporting Information

Nature of WO_x Sites on SiO₂ and their Molecular Structure-Reactivity/Selectivity

Relationships for Propylene Metathesis

Soe Lwin^a, Yuanyuan Li^b, Anatoly I. Frenkel^b, Israel E. Wachs^{a*}

^a *Operando* Molecular Spectroscopy and Catalysis Laboratory, Department of Chemical Engineering, Lehigh University, Bethlehem, PA 18015, USA

^b Department of Physics, Yeshiva University, New York, NY 10016, USA

*Corresponding author: iew0@lehigh.edu

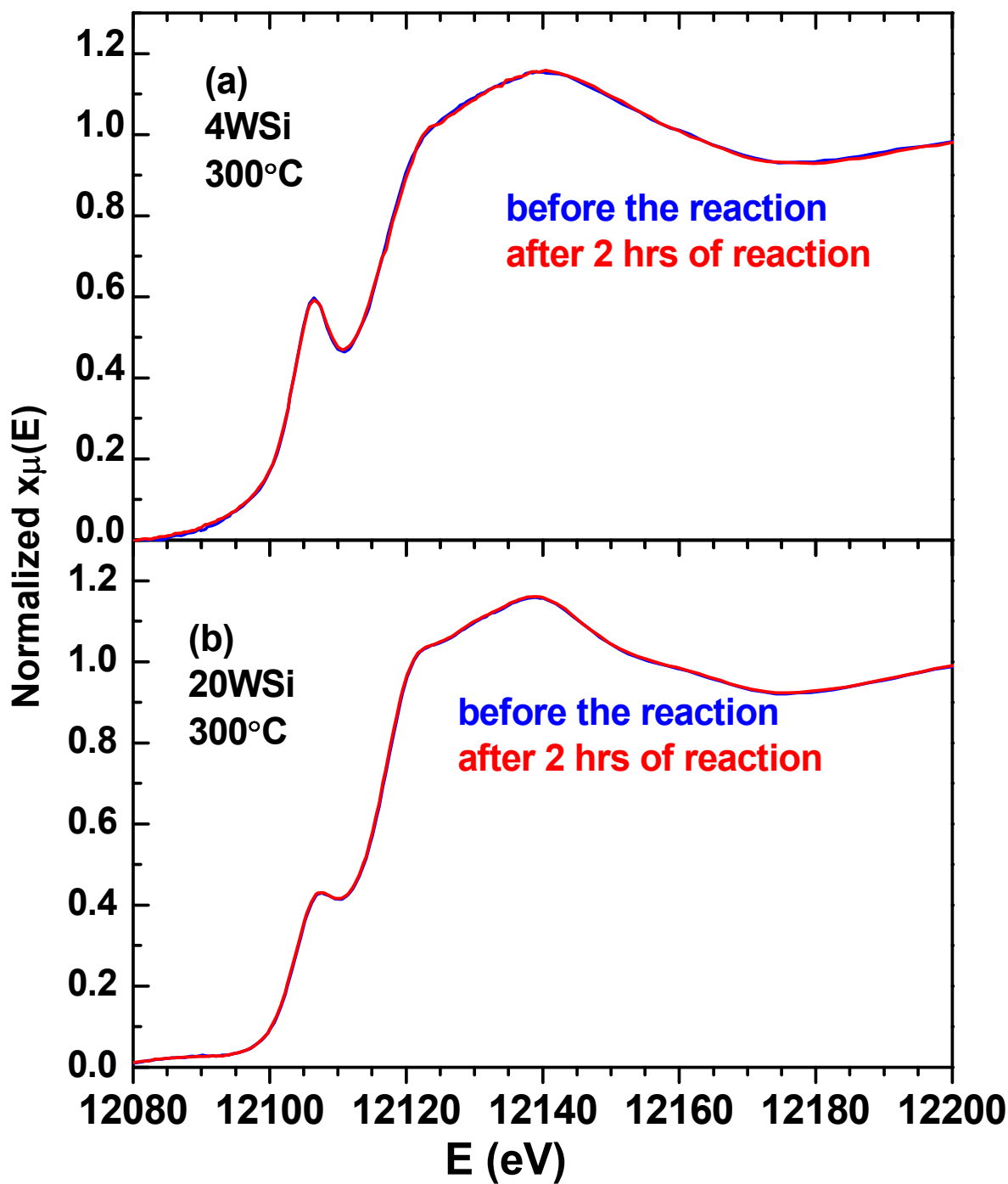


Figure S1. *In situ* W L₁-edge XANES spectra of the (a) 4% and (b) 20% supported WO_x/SiO₂ catalysts before and during reaction at 300°C.

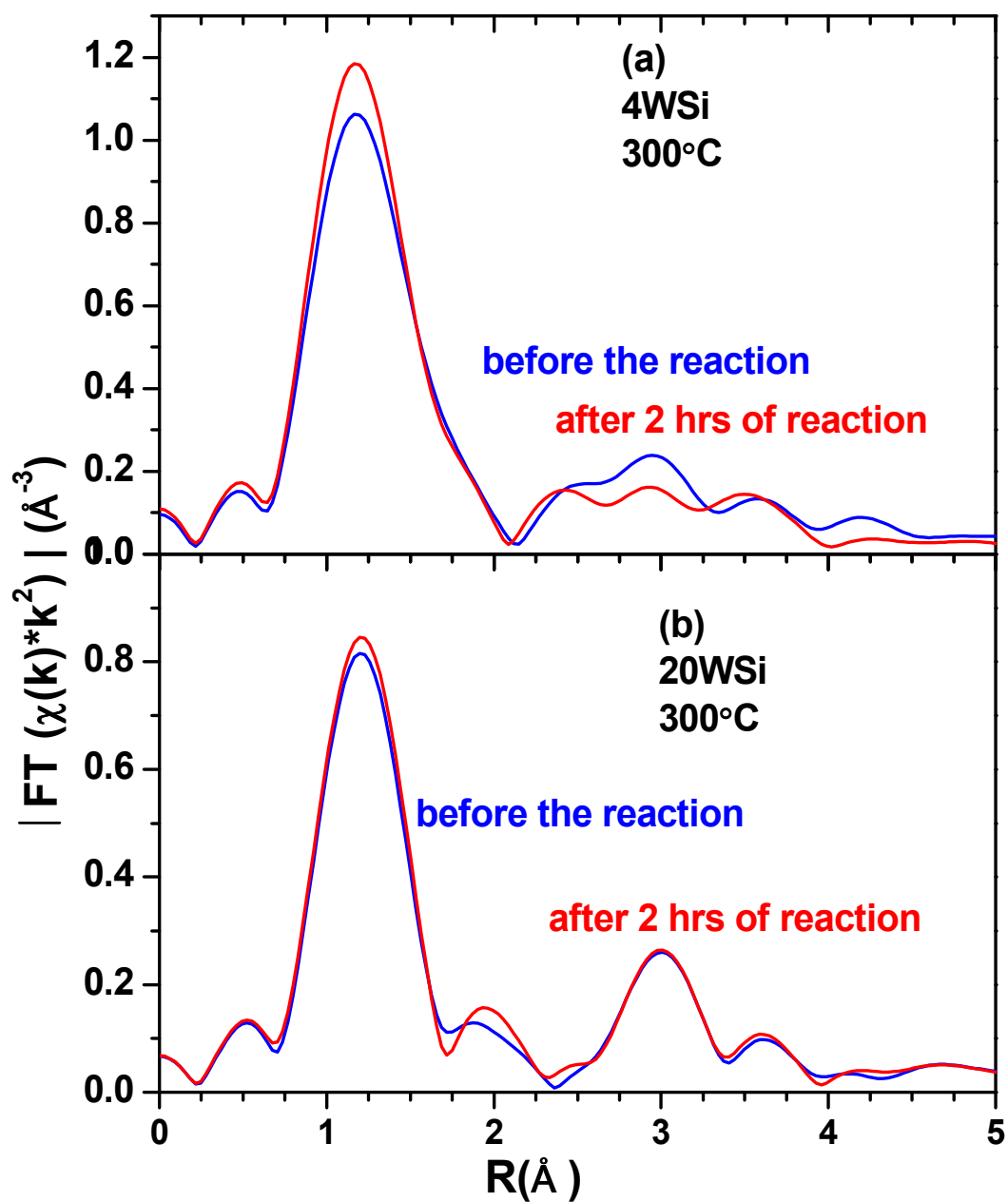


Figure S2. Magnitudes of Fourier-transformed k^2 -weighted *in situ* W L_1 -edge EXAFS spectra in non-phase-corrected R space for the (a) 4% and (b) 20% catalysts before (blue) and during reaction (red) at 300°C.

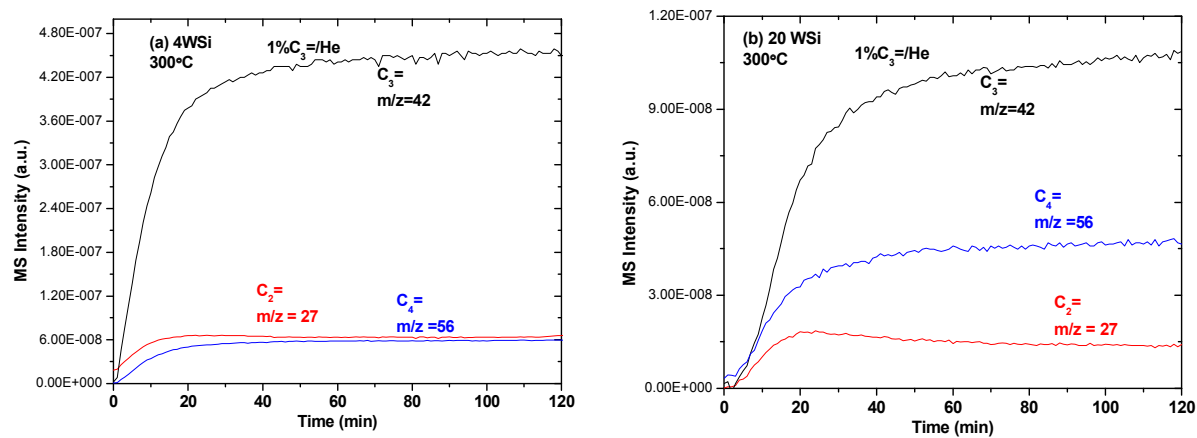


Figure S3. *Operando* MS spectra for the (a) 4% and (b) 20% catalyst which were simultaneously collected along with XANES/EXAFS measurements.

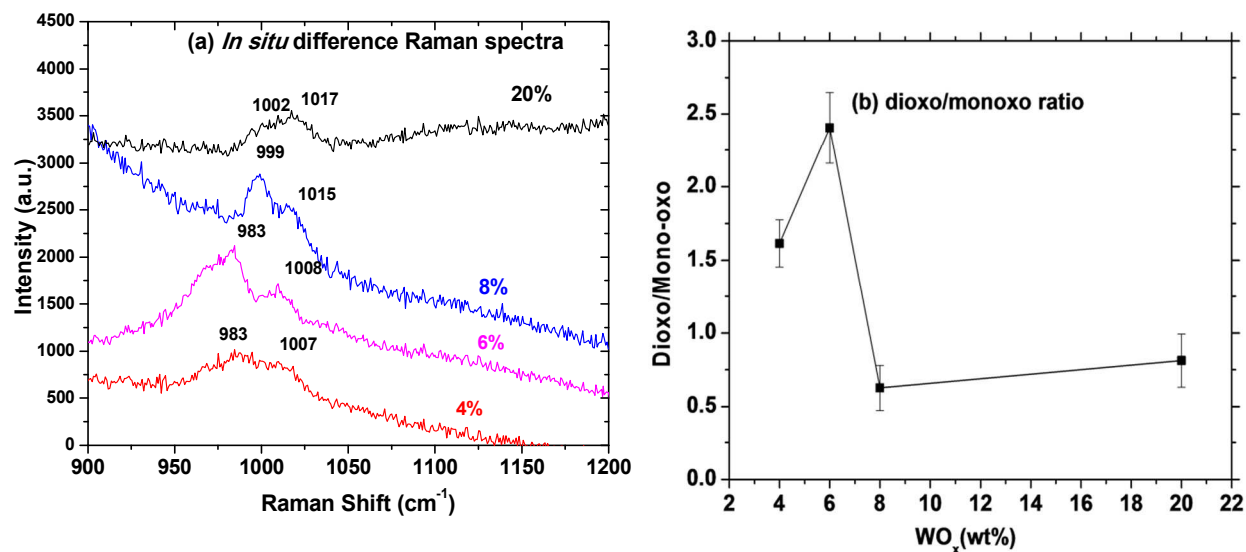


Figure S4. (a) *In situ* difference Raman spectra (442 nm) of the supported WO_x/SiO_2 catalysts under dehydrated conditions (flowing O_2/Ar at 300°C). The SiO_2 spectrum was subtracted from all of the spectra. (b) The ratio of dioxo/mono-oxo obtained from integration of their respective raw Raman bands.

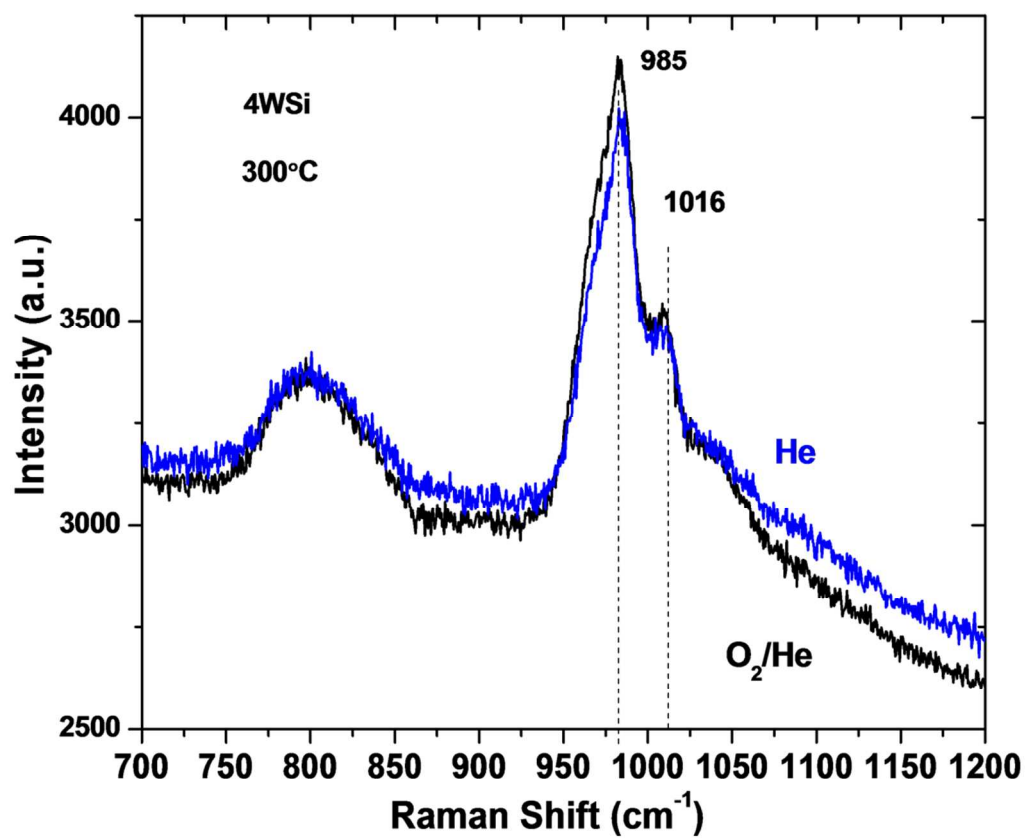


Figure S5. *In situ* Raman spectra of supported 4%WO_x/SiO₂ catalyst at 300°C in flowing O₂/He (30 minutes) or He (30 minutes).

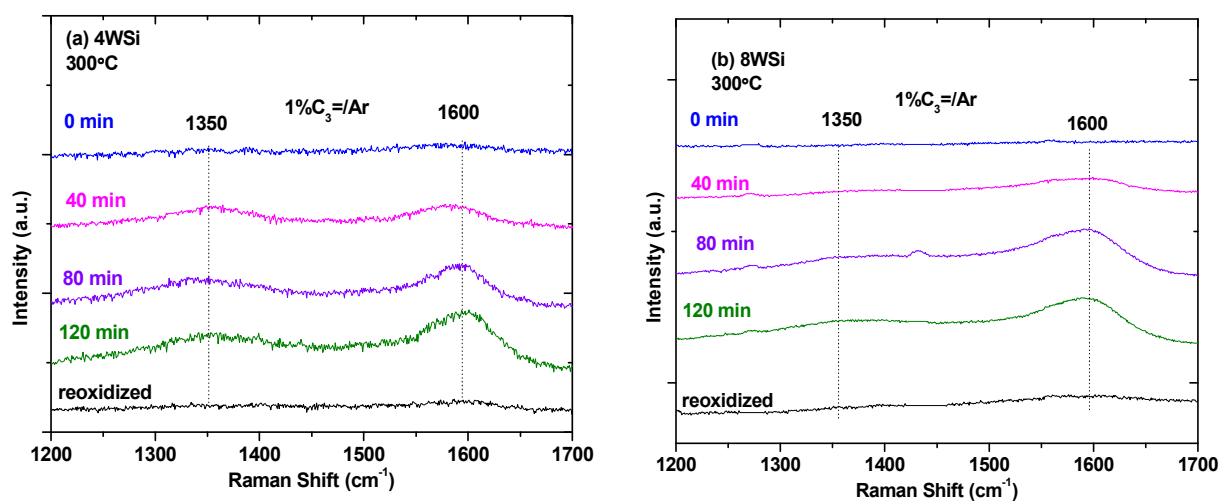


Figure S6. *Operando* Raman spectra for the (a) 4% and (b) 8% catalysts in the 1200-1700 cm^{-1} range showing formation of some coke on the catalysts.

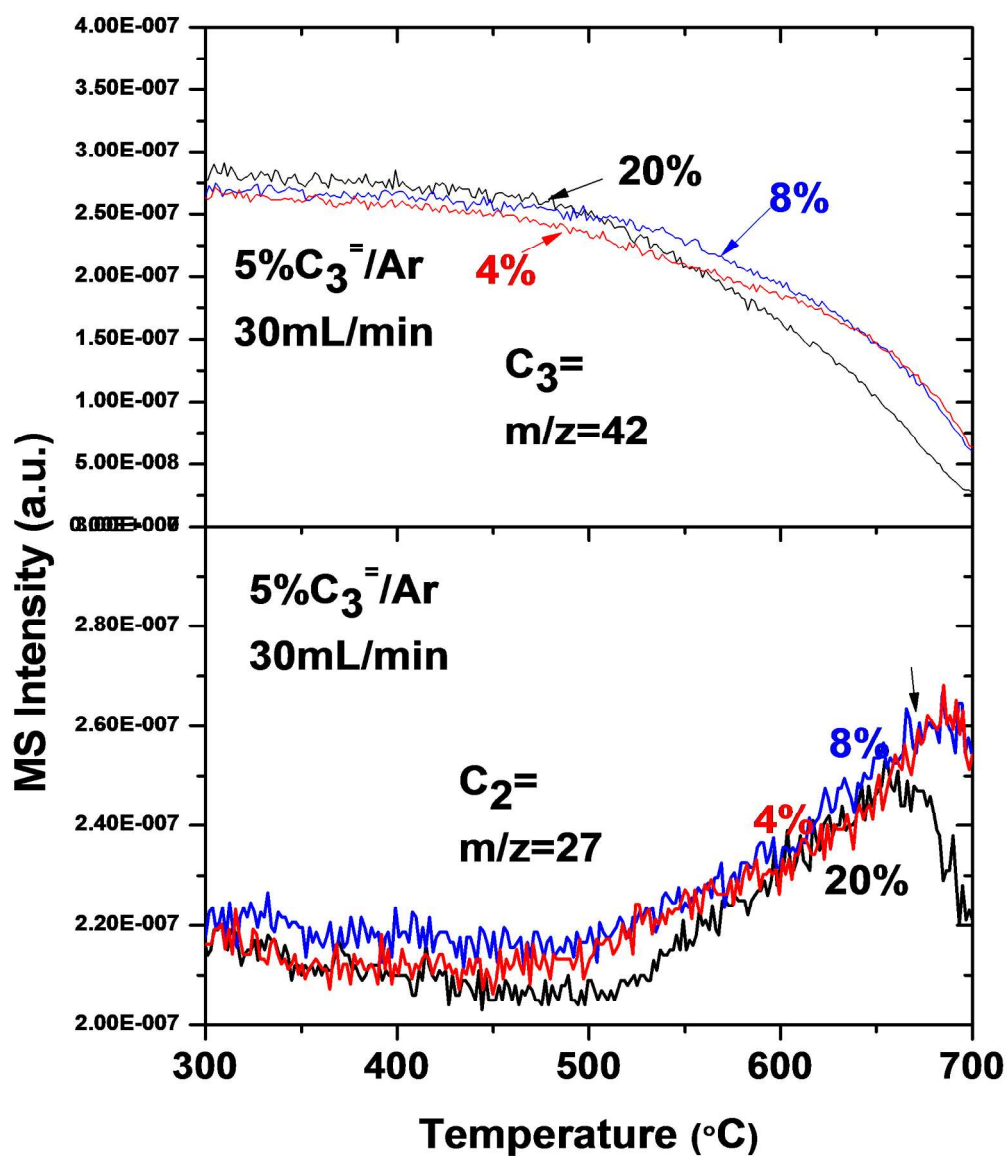


Figure S7. The $C_3=$ and $C_2=$ profiles during $C_3=/Ar$ -TPSR as a function of WO_x loadings (correspond to Figures 9 and 10 in the main text).

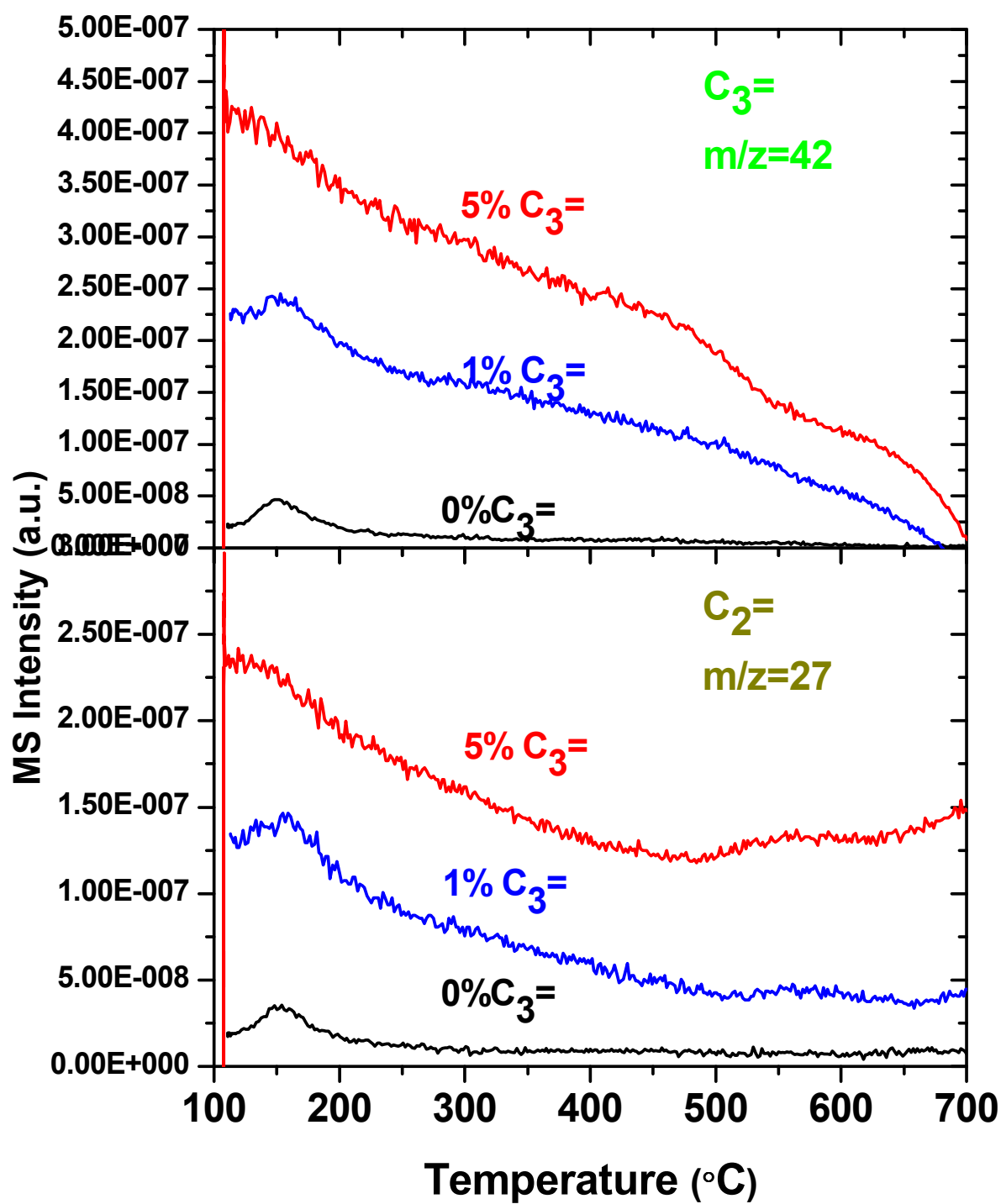


Figure S8. C₃= and C₂= profiles in flowing 0-5% C₃= after 500°C C₃= treatment and 100°C C₃= adsorption