Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Supporting Information

# Surface chemistry of propanal, 2-propenol, and 1-propanol on Ru(001)

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**Contents**

1. TPRS Yields

The TPRS yields listed in Table S1 were calculated using a previously described approach.[1]

**Table S1.** Yields in units of × $10^{-3}$ ML of the products observed with TPRS following exposure to 2-propenol, propanal, and 1-propanol

| Compound | Exposure (L) | Product and Yield × $10^{-3}$ ML | | | | |
|---|---|---|---|---|---|---|
| | | CO | 2-Propenol | Propanal | 1-Propanol | Propene |
| 2-Propenol | 1.0 | 50.0 | 11.0 | 13.9 | 7.13 | 12.7 |
| Propanal | 1.0 | 60.30 | 0 | 18.8 | 0.22 | 0 |
| 1-Propanol | 1.0 | 58.5 | 0 | 11.1 | 150 | 0 |

2. Selected TPR spectra – before and after deconvolution

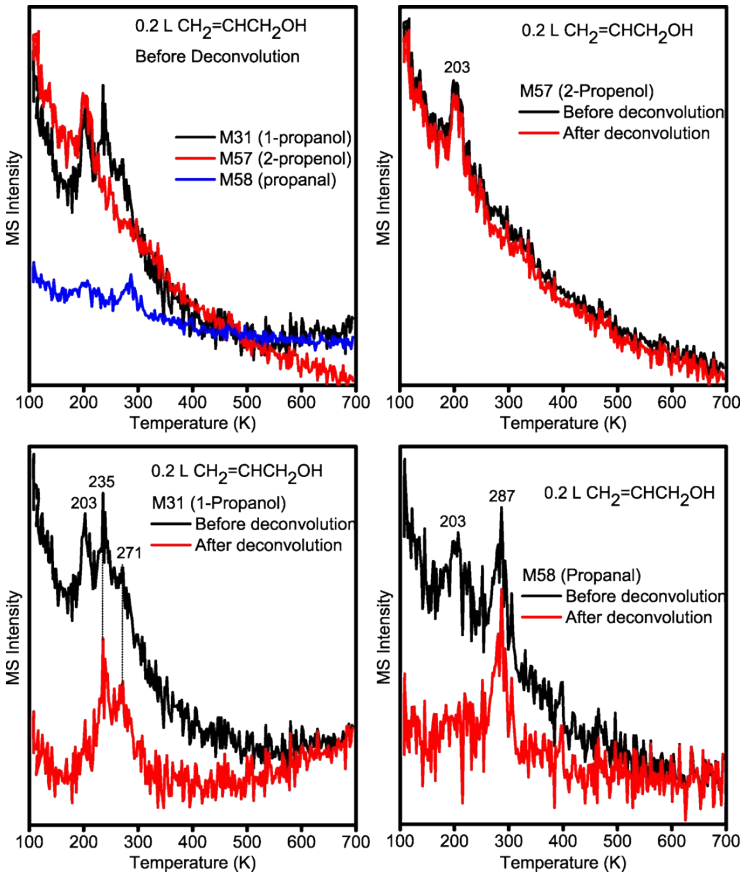


**Figure S1**. Raw and deconvoluted TPR spectra for masses 57 amu (2-propenol), 31 amu (1-propanol), and 58 amu (propanal) after exposing the Ru(001) surface to 0.2 L of 2-propenol.

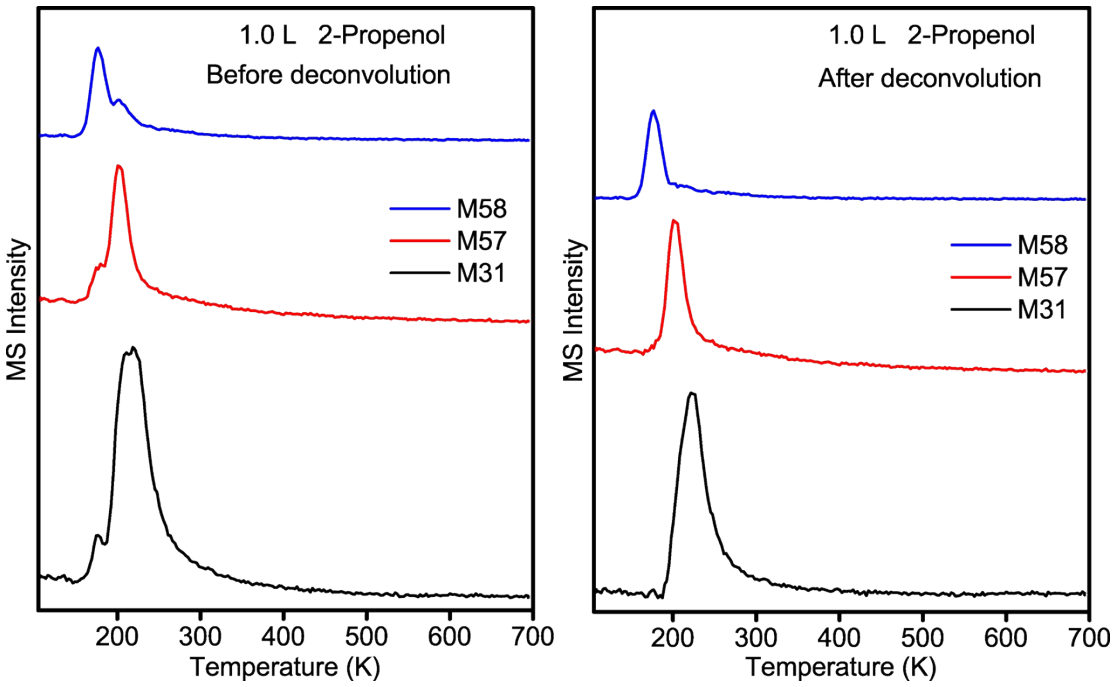


**Figure S2.** Raw and deconvoluted TPR spectra for masses 58 amu (propanal), 57 amu (2-propenol), and 31 amu (1-propanol) obtained after exposing the Ru(001) surface to 1.0 L of 2-propenol.

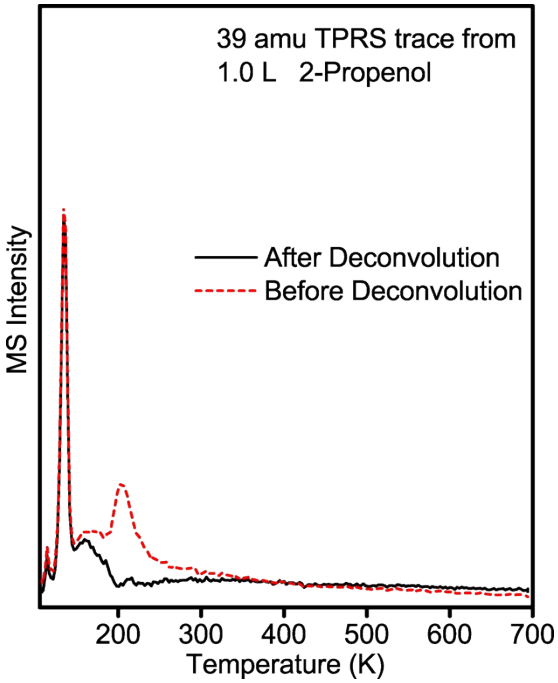


**Figure S3**. Raw and deconvoluted TPRS spectra for 39 amu (propene) obtained after exposing the Ru(001) surface to 1.0 L of 2-propenol.

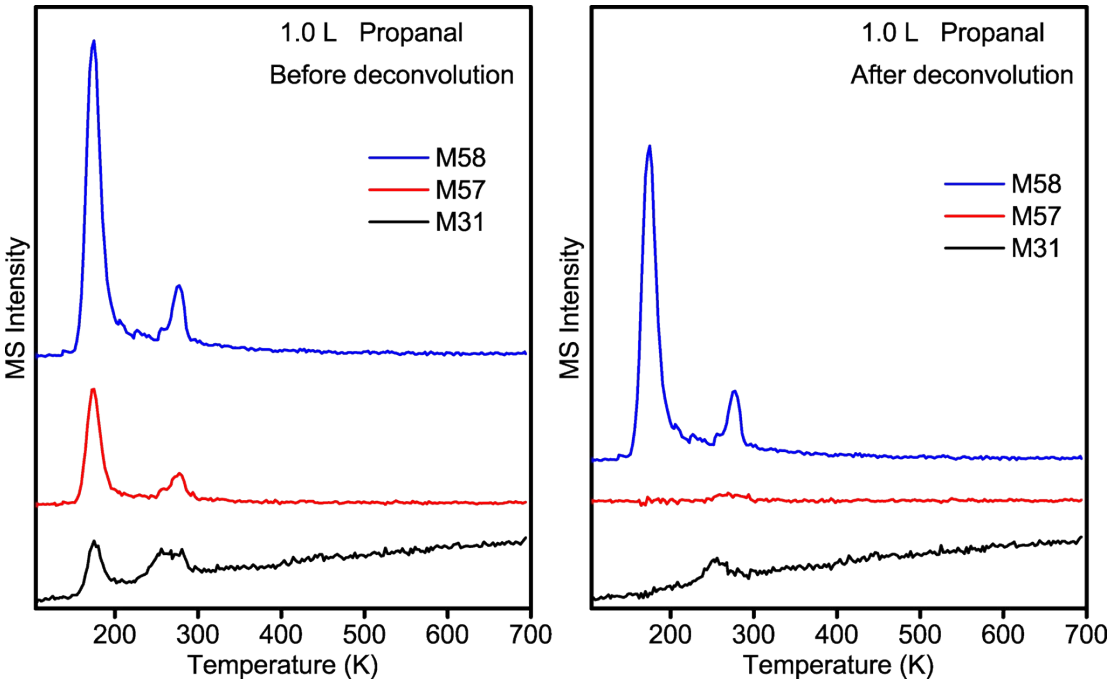


**Figure S4**. Raw and deconvoluted TPRS spectra for masses 58 amu (propanal), 57 amu (2-propenol), and 31 amu (1-propanol) obtained after exposing the Ru(001) surface to 1.0 L of propanal.

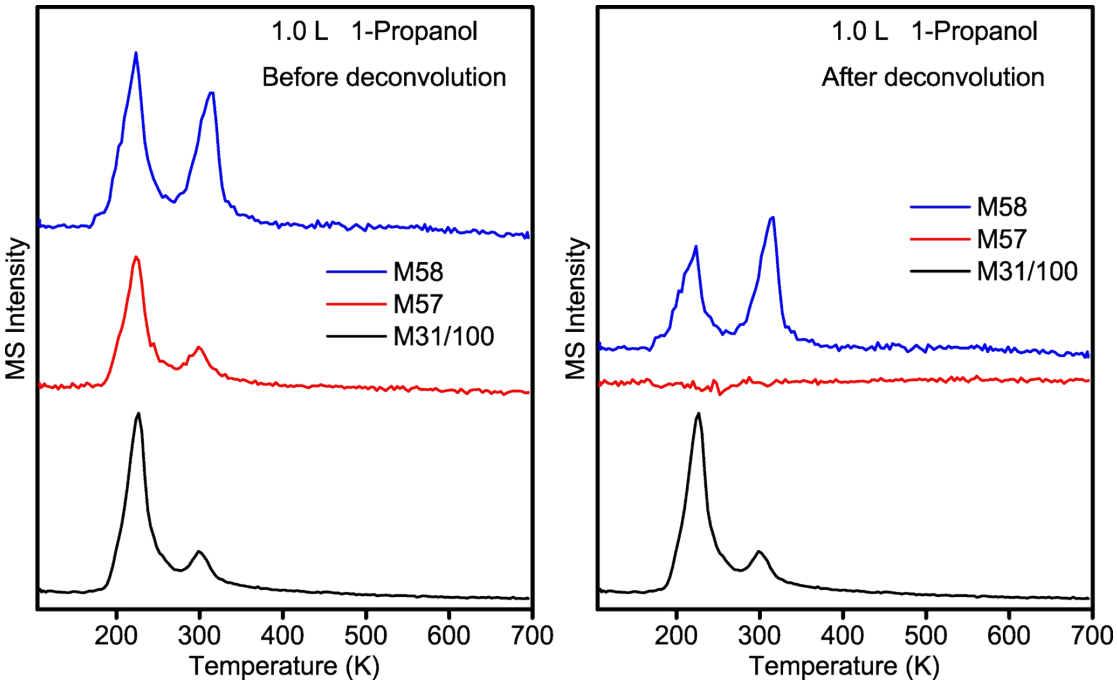


**Figure S5**. Raw and deconvoluted TPRS spectra for masses 58 amu (propanal), 57 amu (2-propenol), and 31 amu (1-propanol) obtained after exposing the Ru(001) surface to 1.0 L of 1-propanol.

3. RAIR spectra of 2-propenol, propanal, and 1-propanol at different exposures

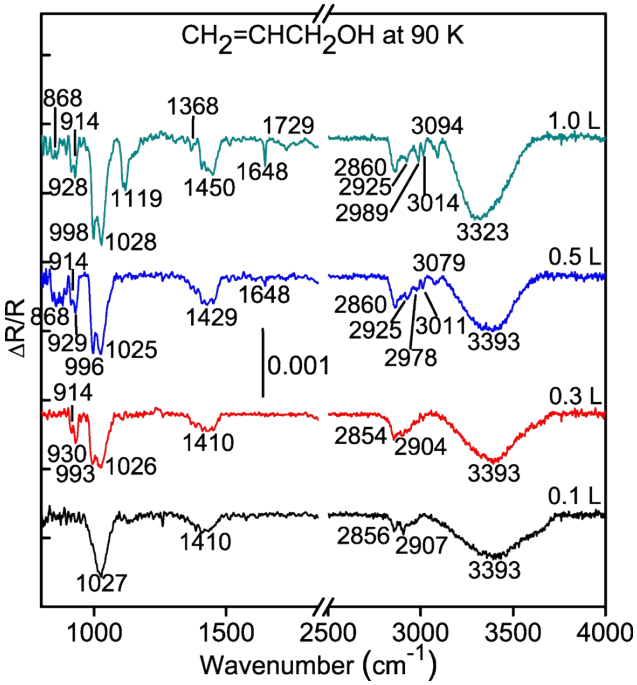


**Figure S6**. RAIR spectra of 0.1 to 1.0 L 2-propenol taken at 90 K on the clean Ru(001) surface.

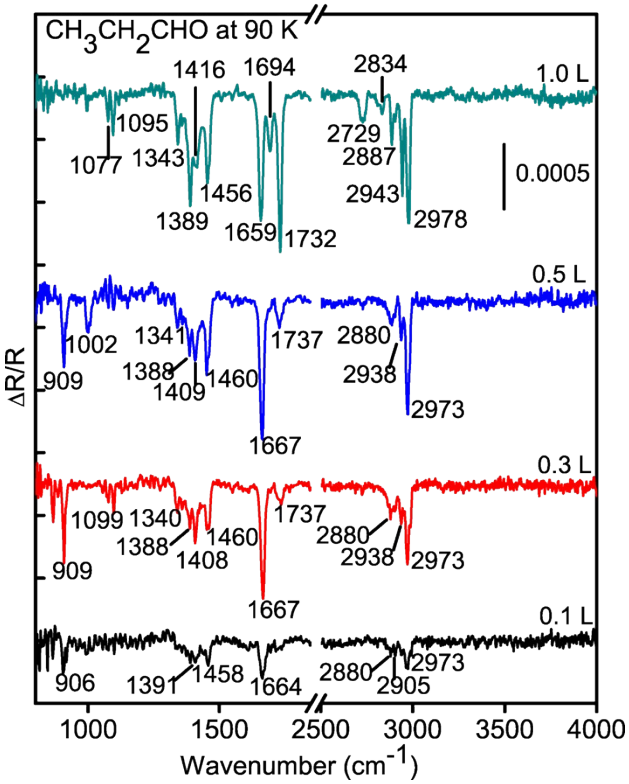


**Figure S7**. RAIR spectra of 0.1 to 1.0 L propanal taken at 90 K on the clean Ru(001) surface.

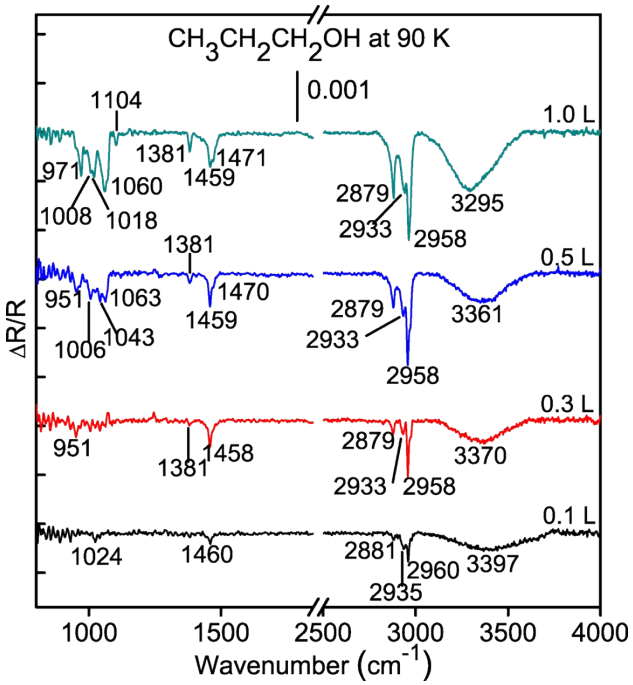


**Figure S8**. RAIR spectra of 0.1 to 1.0 L 1-propanol taken at 90 K on the clean Ru(001) surface.

References

1. D. A. Esan, Y. Ren, X. Feng and M. Trenary, *J. Phys. Chem. C*, 2016, DOI: 10.1021/acs.jpcc.6b12678.