SUPPLEMENTAL INFORMATION

Correlating the Surface Chemistry of C_2 and C_3 Aldoses with a C_6 Sugar: Reaction of Glucose, Glyceraldehyde and Glycolaldehyde on Pd(111)

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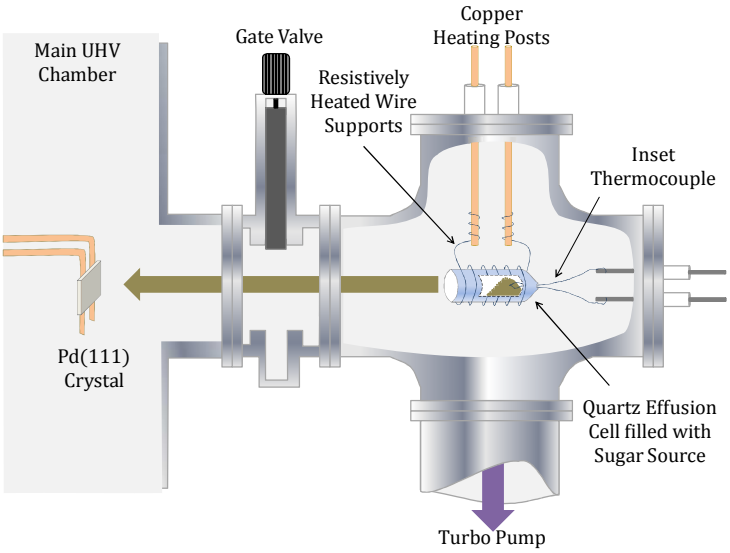

Figure S1: Schematic of glucose/glyceraldehyde molecular beam dosing apparatus.

MOLECULAR DOSING EXPERIMENTS

Initial TPD studies focused on identifying the dosage required to produce a saturation coverage of each reactant on Pd(111) and to further verify the production of glyceraldehyde and glucose vapors from the effusion cells. TPD spectra as a function of exposure for glycolaldehyde, glyceraldehyde, and glucose are presented in Figure S2. The glycolaldehyde spectra in Figure S2a show the emergence of the parent mass m/e 60 at 170 K for exposures greater than ~0.5 L. In addition to m/e 60, identical peaks for the other primary cracking fragments of glycolaldehyde, i.e. m/e 32, 31, and 29, were also observed (not shown in the figure) with relative intensities consistent with those in the mass spectrum of glycolaldehyde in the NIST mass spectrometry database. The m/e 60 peak can, therefore, be assigned to desorption of molecular glycolaldehyde. Since the onset of desorption of the molecular species occurred for a 0.5 L dose, this dose was used in the TPD and HREELS experiments described below which focused on characterizing the surface reactions of chemisorbed glycolaldehyde.

The analogous data for glyceraldehyde is shown in Figure S2b. In this case m/e 61, which is a primary cracking fragment, was used to monitor for glyceraldehyde desorption. The molecular desorption spectra for glyceraldehyde were slightly more complex than those for glycolaldehyde with

two separate desorption peaks at 214 and 281 K emerging for exposures greater than 0.25 L, with the higher temperature peak increasing in size more rapidly with coverage. While additional study is needed to determine the origin of each peak, it is possible that the peaks are due to the presence of both monomers and dimers in the adsorbed multilayers, with the dimers dissociating and desorbing at the higher temperature. Based on these data, a 0.25 L dose was chosen for use in subsequent TPD and HREELS experiments which focused on the reaction of glyceraldehyde on Pd(111).

As expected, the TPD results for glucose on Pd(111) in Figure S2c show that it is less volatile than the other aldoses with the molecular desorption peak appearing at 325 K. The figure shows data for m/e 73, with identical peaks also observed for the other primary cracking fragments for glucose reported in the NIST mass spectrometry database (e.g., m/e 61, 60, 43, and 31). Based on these data, a 0.4 L dose was chosen for use in subsequent TPD and HREELS experiments which focused on the reaction of chemisorbed glucose on Pd(111).

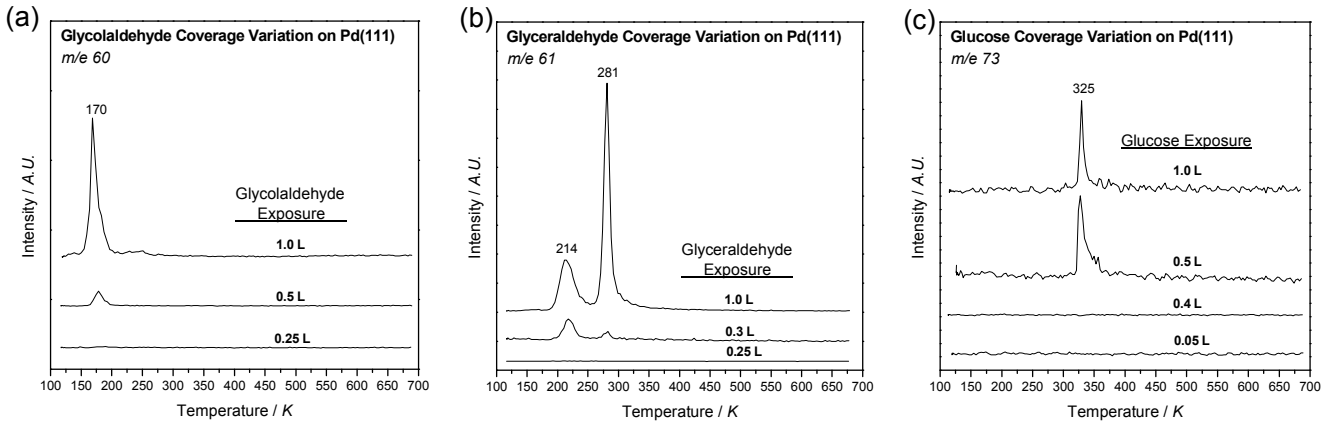

Figure S2: Coverage variation TPD for (a) glycolaldehyde, (b) glyceraldehyde and (c) glucose.