Supporting Information

Kinetics and mechanism of aspartic acid adsorption and its explosive decomposition on Cu(100)

*[1]Burcu Karagoz, [1]Aaron Reinicker, and [1,2]Andrew J. Gellman**

[1]Department of Chemical Engineering

[2]W.E. Scott Institute for Energy Innovation

5000 Forbes Ave., Pittsburgh, PA 15213, USA

* Corresponding author: 412-268-3848, gellman@cmu.edu

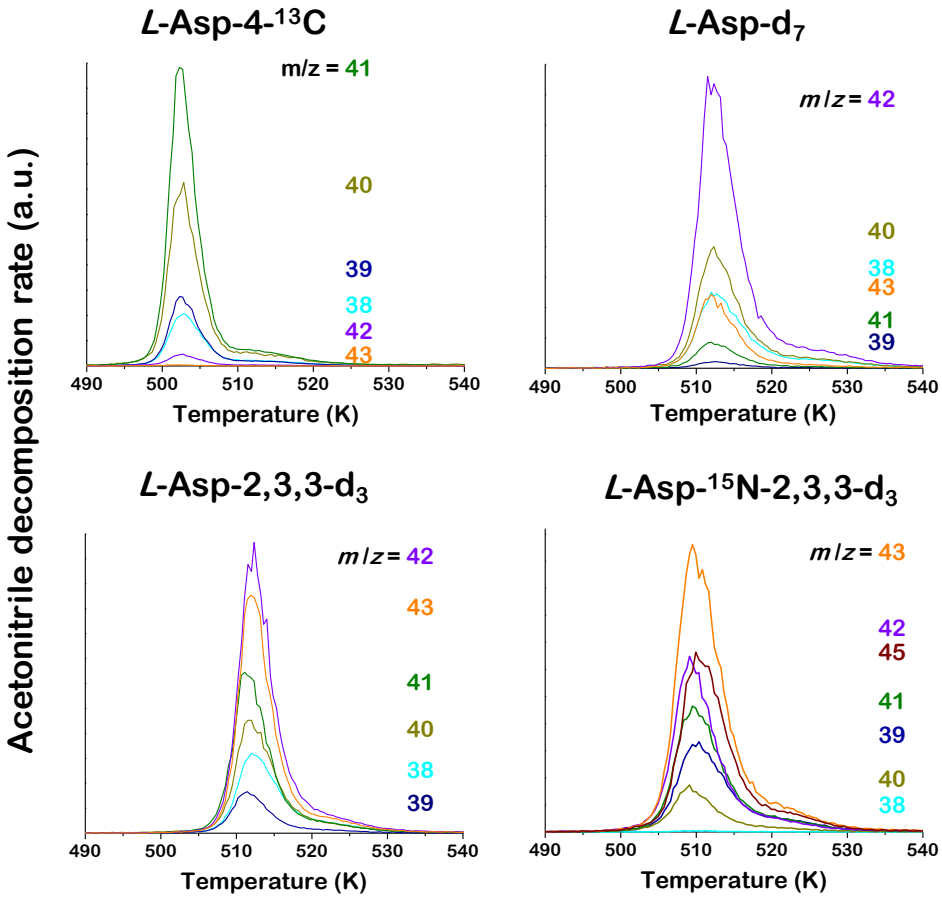

Figure S1. Fragments of acetonitrile desorption rate at 0.5 K/s heating rate. TPR spectra at the top left corner shows *L*-Asp-4-^{13}C/Cu(100). TPR spectra at the top right corner shows *L*-Asp-d_7/Cu(100). TPR spectra at the bottom left corner shows *L*-Asp-2,3,3-d_3/Cu(100). Bottom TPR spectra at the bottom right corner shows *L*-Asp-^{15}N-2,3,3-d_3/Cu(100). The signals are collected at *m/z* = 38 ($N{\equiv}CC^+$), 39 ($N{\equiv}CCH^+$, $^{15}N{\equiv}CC^+$), 40 ($N{\equiv}CCH_2^+$, $N{\equiv}CCD^+$, $^{15}N{\equiv}CCH^+$), 41 ($N{\equiv}CCH_3$, $N{\equiv}CCDH^+$, $^{15}N{\equiv}CCH_2^+$, $^{15}N{\equiv}CCD^+$), 42 ($N{\equiv}CCDH_2$, $N{\equiv}CCD_2^+$, $^{15}N{\equiv}CCH_3$, $^{15}N{\equiv}CCDH^+$), 43 ($N{\equiv}CCD_2H$, $^{15}N{\equiv}$ $CCDH_2$, $^{15}N{\equiv}CCD_2^+$), and 45 ($^{15}N{\equiv}CCD_3$).

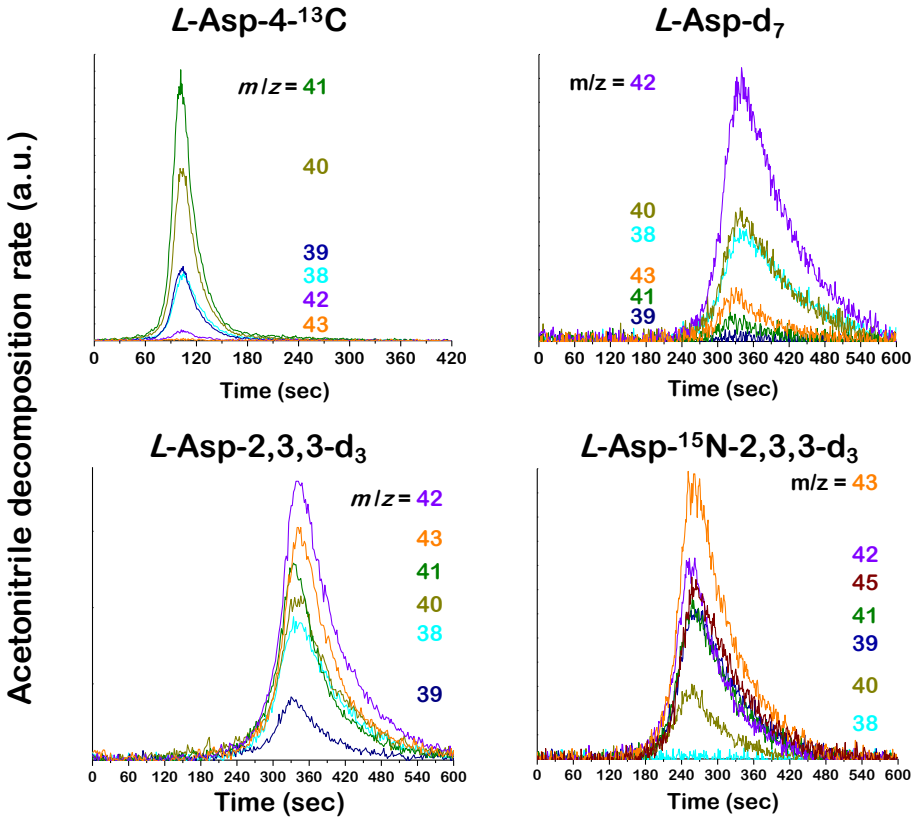

Figure S2. Fragments of acetonitrile desorption rate at isothermal temperature. TPR spectra at the top left corner shows *L*-Asp-4-^{13}C/Cu(100). TPR spectra at the top right corner shows *L*-Asp-d$_7$/Cu(100). TPR spectra at the bottom left corner shows *L*-Asp-2,3,3-d$_3$/Cu(100). Bottom TPR spectra at the bottom right corner shows *L*-Asp-^{15}N-2,3,3-d$_3$/Cu(100). The signals are collected at *m/z* = 38 (N≡CC$^+$), 39 (N≡CCH$^+$, ^{15}N≡CC$^+$), 40 (N≡CCH$_2^+$, N≡CCD$^+$, ^{15}N≡CCH$^+$), 41 (N≡CCH$_3$, N≡CCDH$^+$, ^{15}N≡CCH$_2^+$, ^{15}N≡CCD$^+$), 42 (N≡CCDH$_2$, N≡CCD$_2^+$, ^{15}N≡CCH$_3$, ^{15}N≡CCDH$^+$), 43 (N≡CCD$_2$H, ^{15}N≡ CCDH$_2$, ^{15}N≡CCD$_2^+$), and 45 (^{15}N≡CCD$_3$). Isothermal temperature is 480 K.

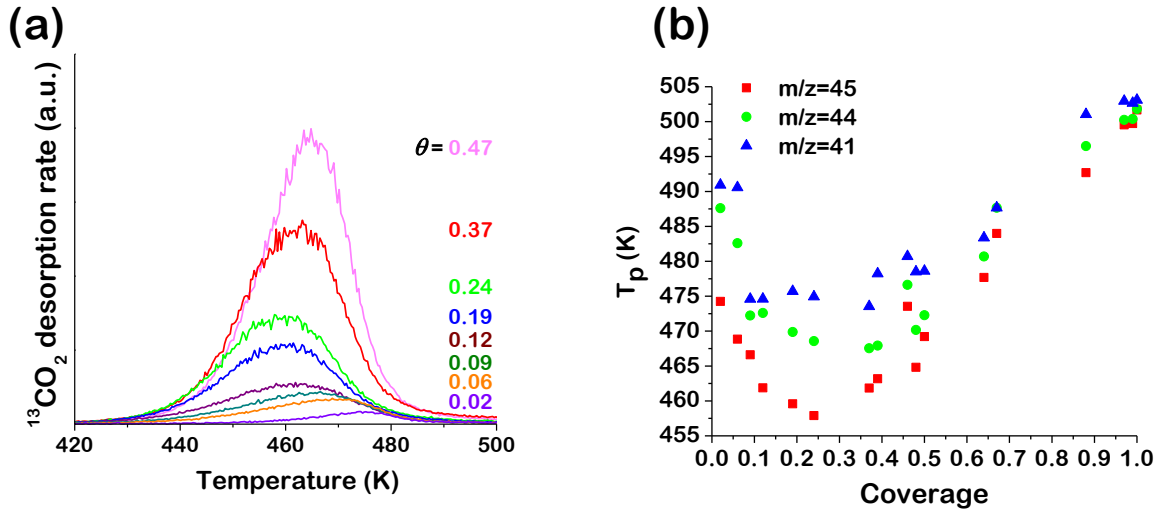

Figure S3. (a) Measured $^{13}CO_2$ desorption rate during *L*-Asp-4-^{13}C decomposition on Cu(100) at θ=0.02-0.47. (Right) Peak temperature of $^{13}CO_2$ (*m/z*=45), CO_2 (*m/z*=44), and N≡CCH_3 (*m/z*=41) with increasing coverages of Asp on Cu(100). For decomposition products of Asp, peak temperature decreases over the coverage range $0.02 \leq \theta \leq 0.22$, then increases with increasing coverages of Asp.