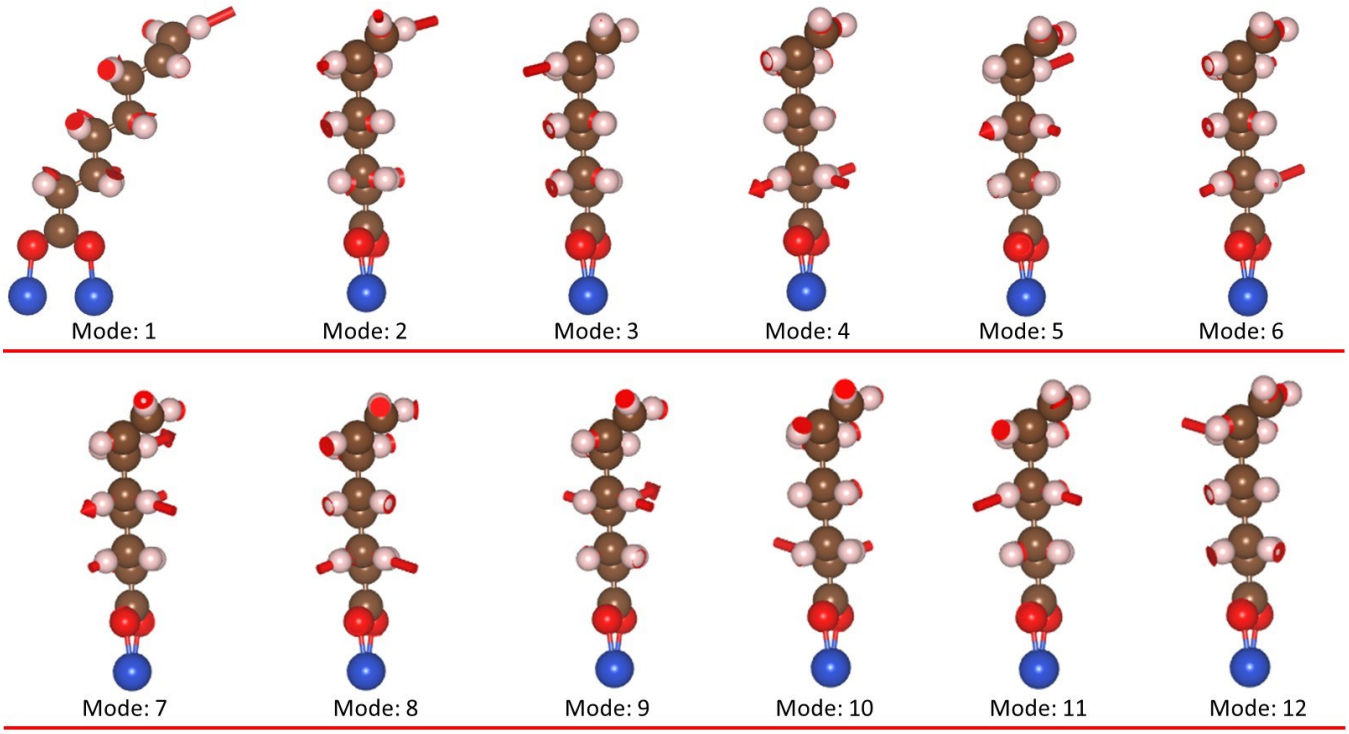
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

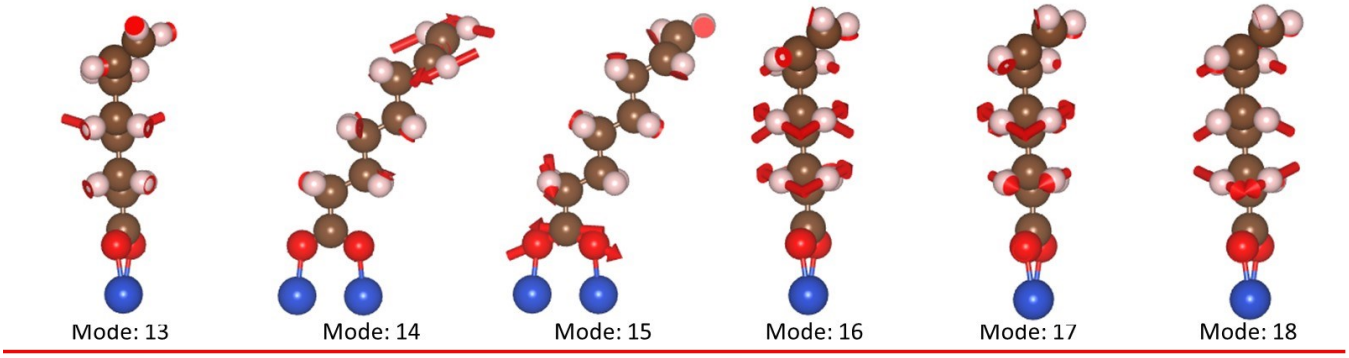
Adsorption and Structural Changes of 7-octenoic Acid on Copper

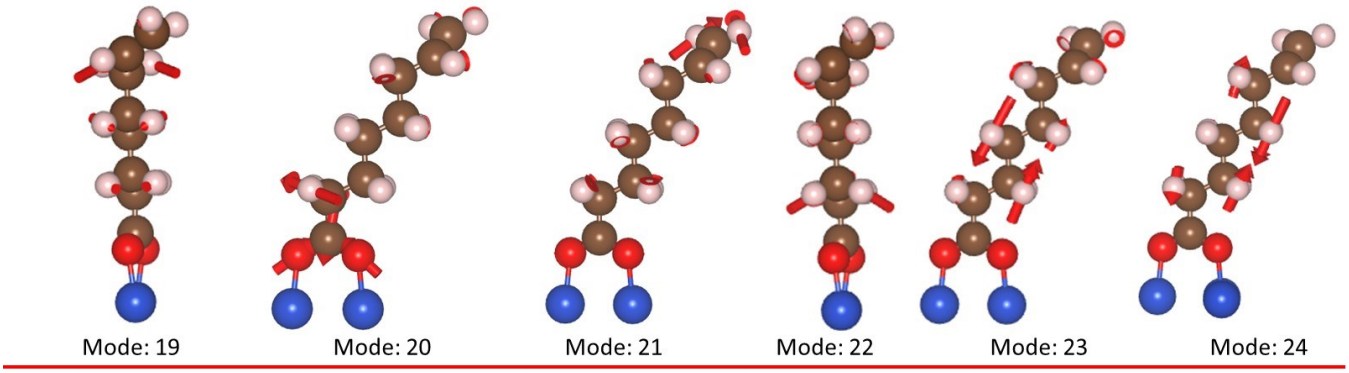
Robert Bavisotto,[1] Resham Rana,[1] Nicholas Hopper,[1] Dustin Olson, and Wilfred T Tysoe [1] *

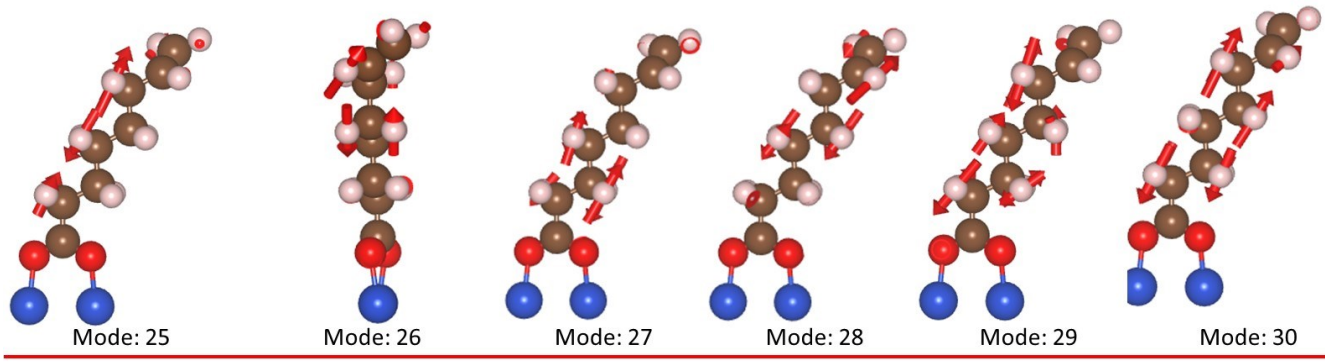
[1] *Department of Chemistry and Biochemistry and laboratory for Surface Studies, University of Wisconsin-Milwaukee, Milwaukee, WI 53211, USA*

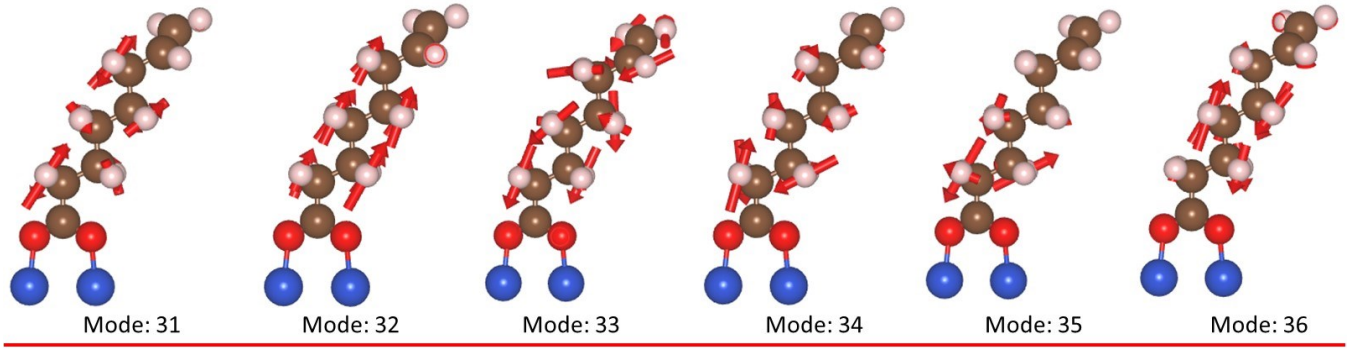
Supplemental Information

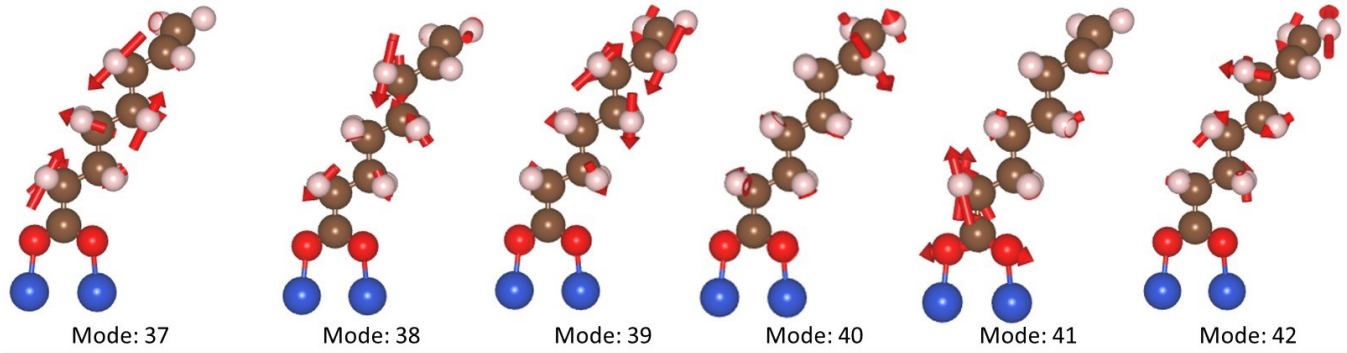


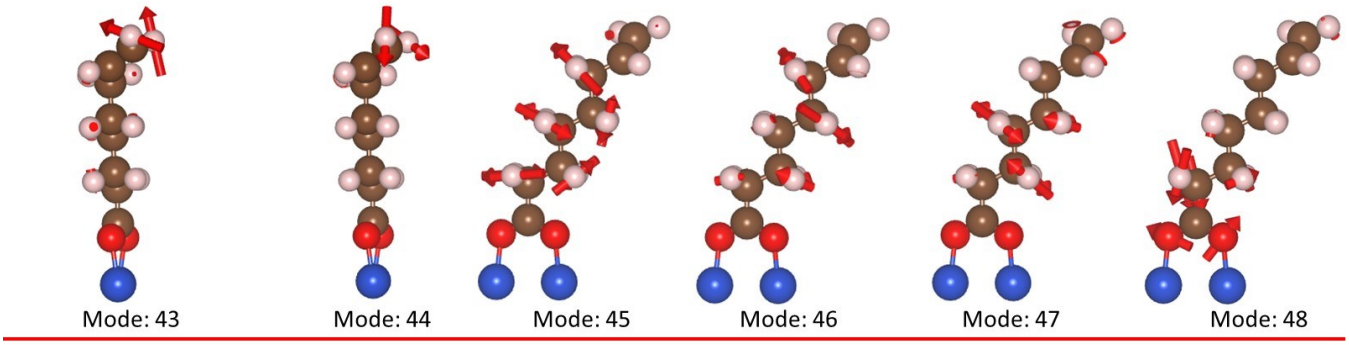

Mode: 13
Mode: 14
Mode: 15
Mode: 16
Mode: 17
Mode: 18

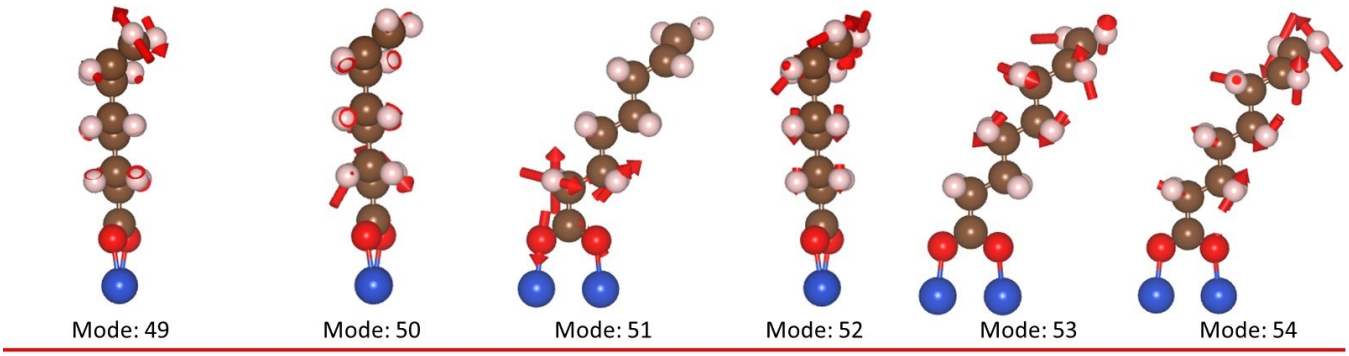

Mode: 19
Mode: 20
Mode: 21
Mode: 22
Mode: 23
Mode: 24

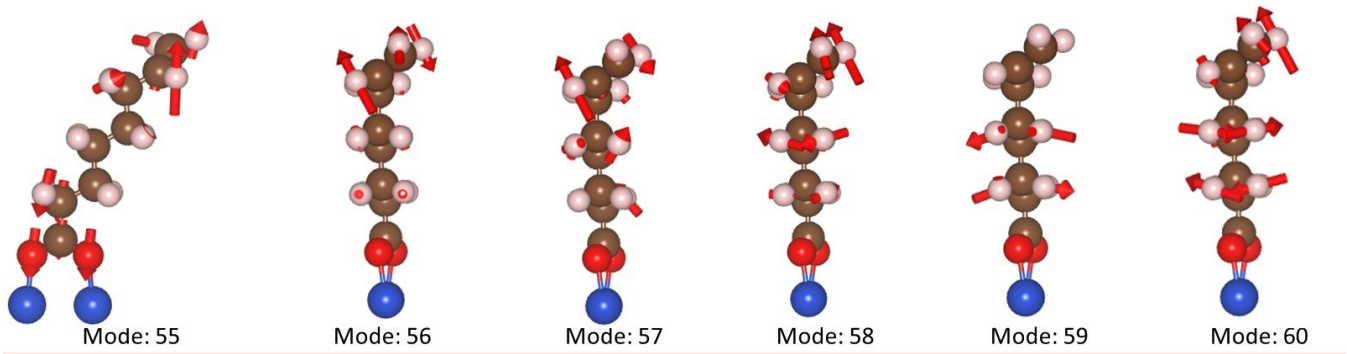

Mode: 25
Mode: 26
Mode: 27
Mode: 28
Mode: 29
Mode: 30

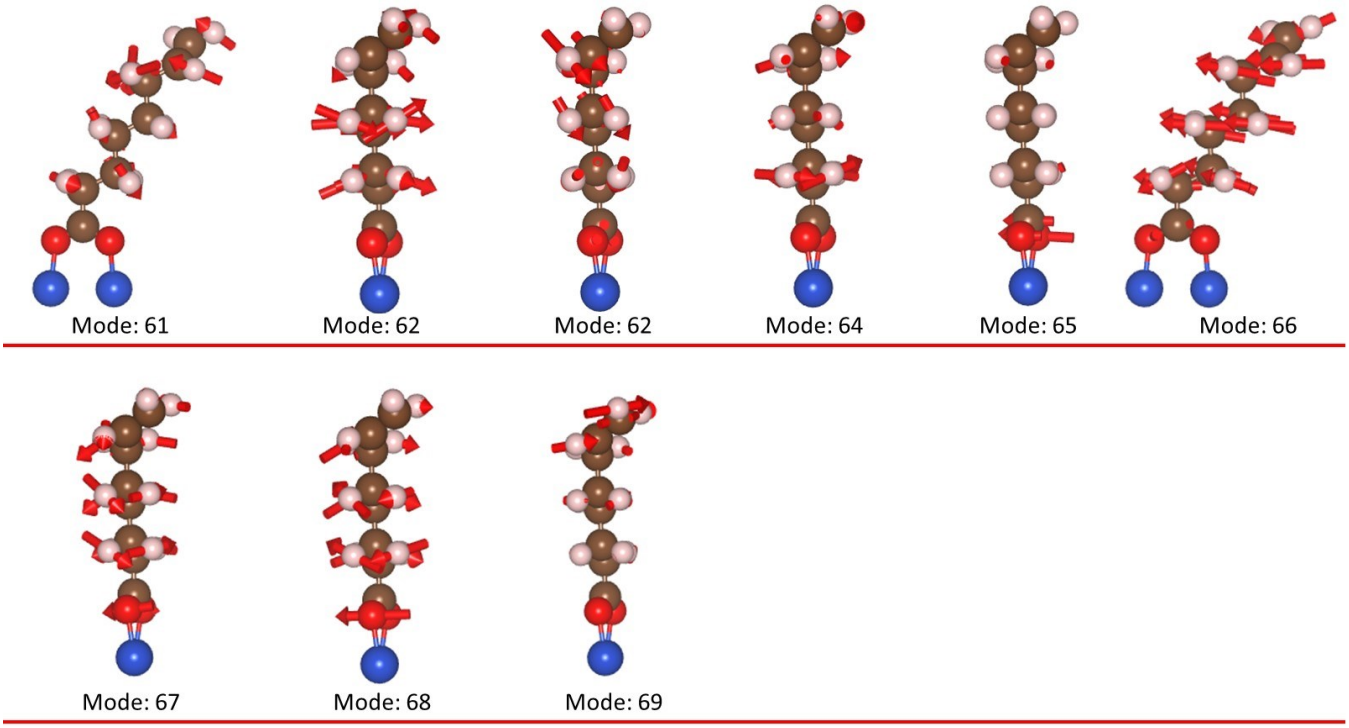

Mode: 31
Mode: 32
Mode: 33
Mode: 34
Mode: 35
Mode: 36


Mode: 37
Mode: 38
Mode: 39
Mode: 40
Mode: 41
Mode: 42


Mode: 43
Mode: 44
Mode: 45
Mode: 46
Mode: 47
Mode: 48


Mode: 49
Mode: 50
Mode: 51
Mode: 52
Mode: 53
Mode: 54


Mode: 55
Mode: 56
Mode: 57
Mode: 58
Mode: 59
Mode: 60

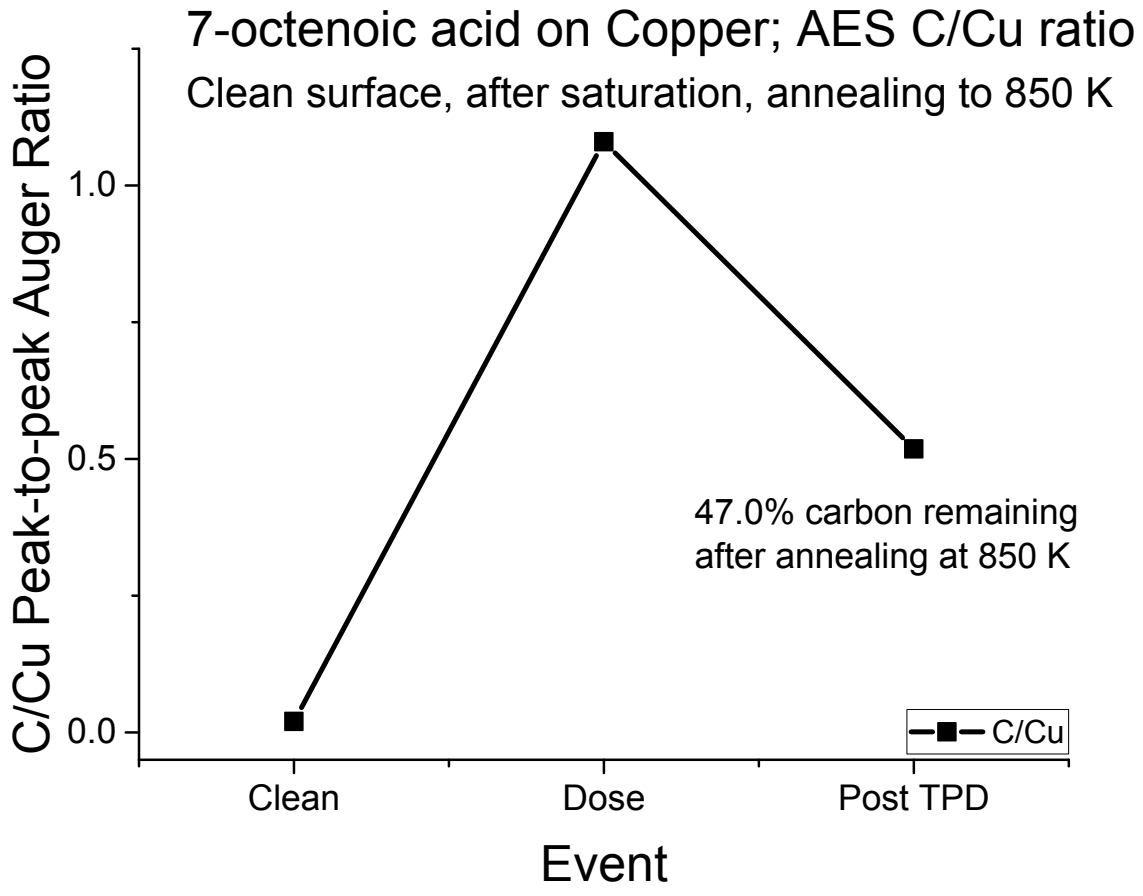


Supplemental Figure 1: Graphical depiction of the atomic displacements for the normal modes of 7-octenoic acid.

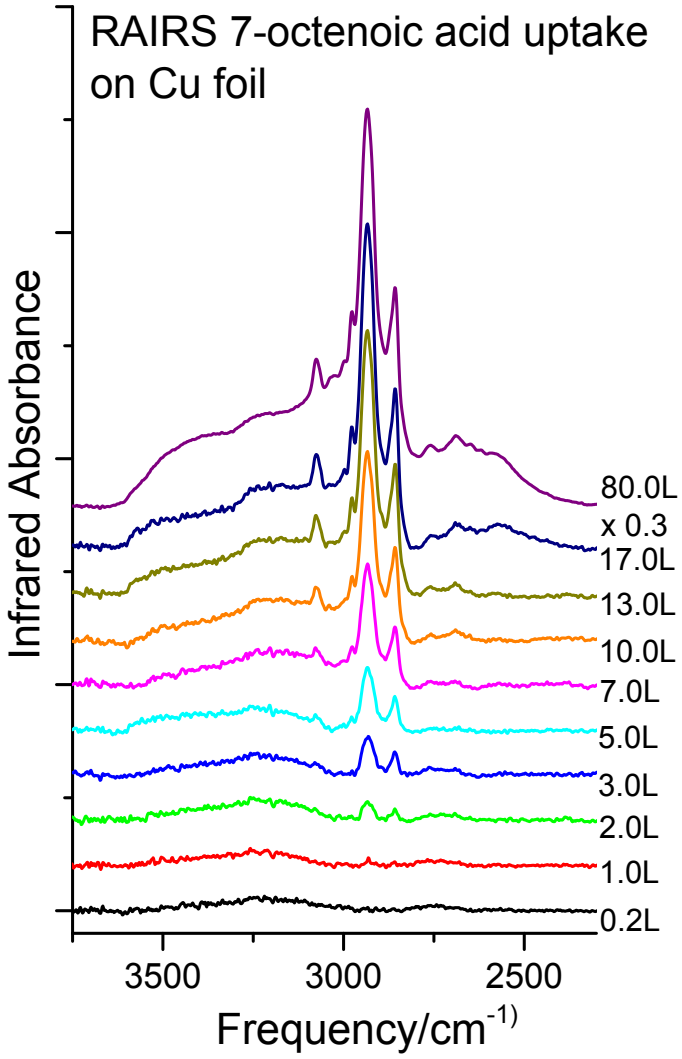
Mode Number	Calculated Frequency/cm^{-1}	7-octenoic acid multilayer/Cu(100)/cm^{-1}	7-octenoic acid annealed multilayer/Cu(100)/cm^{-1}	Assignments
1	3529	3500-2900 Broad		O-H stretch
2	2955	2955	2955	C-H modes
3	2947			
4	2937	2929		C-H modes
5	2914		2020	C-H modes
6	2910			
7	2898			
8	2896			
9	2887			
10	2881			
11	2878		2872	C-H modes
12	2873			
13	2871			
14	2862			
15	2858	2856		C-H modes
16	2854		2853	C-H modes
17	1708	1716	1713	C = O stretch
18	1422	1471	1468	C-H modes
19	1416			
20	1414	1412	1414	C-H modes
21	1407			
22	1400			
23	1394			
24	1392			
25	1363			

26	1327			
27	1326	1327		C-H modes
28	1313			
29	1306			
30	1278	1286		C-H modes
31	1257			
32	1256			
33	1245			
34	1239	1242	1238	
35	1227			
36	1205	1203	1200	
37	1185			
38	1171			
39	1141	1116		C-H modes
40	1092			
41	1068			
42	1055			
43	1041			
44	1038			
45	1022			
46	996			
47	976	966		C-C modes
48	958		939	C-H modes

Supplemental Table 1: Calculated vibrational frequencies of 7-octeoic acid on Cu(100), compared with the results of reflection-absorption infrared spectroscopic measurements.



Supplemental Figure 2: Plot of the C/Cu peak-to-peak ratio of the Auger spectrum of a clean copper surface prior to dosing with 7-octanoic acid, after saturating the copper surface with 7-octanoic acid at 300 K, and after heating the surface to 850 K.



Supplemental Figure 3: Infrared spectra collected using a resolution of 4 cm^{-1} for the adsorption of 7-octenoic acid on Cu(100) at a sample temperature of 90 K as a function of exposure on Langmuirs (L), where the exposures are displaced adjacent to the corresponding spectrum, showing the C–H stretching region.