

Supplementary Information:

Surface Structure and Electron Transfer Dynamics of the Self-Assembly of Cyanide on Au{111}

Andrew I. Guttentag,^{1,2} Tobias Wächter,³ Kristopher K. Barr,^{1,2} John M. Abendroth,^{1,2} Tze-Bin Song,^{1,4} Nichole F. Sullivan,⁵ Yang Yang,^{1,4} David L. Allara,^{*⁵} Michael Zharnikov,^{*³} and Paul S. Weiss^{*^{1,2,4}}

¹California NanoSystems Institute, University of California, Los Angeles, Los Angeles, California 90095, United States

²Department of Chemistry and Biochemistry, University of California, Los Angeles, Los Angeles, California 90095, United States

³Applied Physical Chemistry, Heidelberg University, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany

⁴Department of Materials Science and Engineering, University of California, Los Angeles, Los Angeles, California 90095, United States

⁵Department of Chemistry, Pennsylvania State University, University Park, Pennsylvania 16802, United States

Keywords: self-assembled monolayers, cyanide, gold, self-assembly, scanning tunneling microscopy, charge transfer, electronic coupling, vibrations, nitrile

*Corresponding authors:

E-mail: psw@cnsi.ucla.edu (P.S.W.).

E-mail: dla3@psu.edu (D.L.A.).

E-mail: michael.zharnikov@urz.uni-heidelberg.de (M.Z.).

Infrared Spectroscopy: Comparison of CN monolayers on Au{111} by Attenuated Total Internal Reflection Fourier Transform Infrared Spectroscopy and Polycrystalline Au/Si Using Polarization-Modulated Fourier Transform Infrared Reflection Absorption Spectroscopy

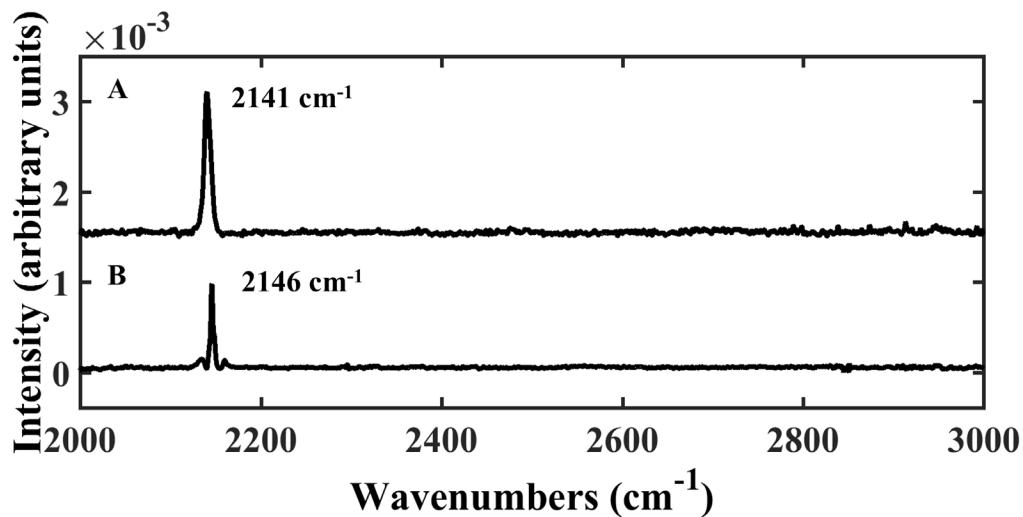


Figure S1. (A) The polarization-modulated Fourier transform infrared reflection absorption spectrum (PM-IRRAS) of CN as-deposited on polycrystalline Au/Si indicating the CN is still primarily upright on the surface without detection of the C-H stretch associated with HCN. (B) The attenuated total internal reflectance Fourier transform infrared spectrum of as-deposited CN on Au{111} showing the multiplet not detected by PM-IRRAS and a blue shift of 5 cm⁻¹.

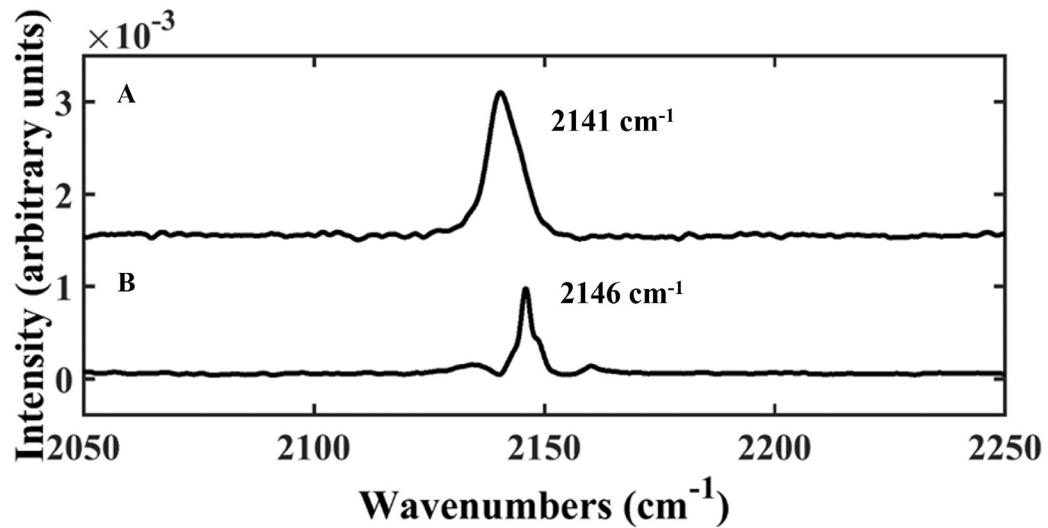


Figure S2. Detail of the (A) CN region from the polarization-modulated Fourier transform infrared reflection absorption spectrum of CN as-deposited on polycrystalline Au/Si and (B) the attenuated total internal reflectance Fourier transform infrared spectrum of as-deposited CN on Au{111}.