

Tunable Interfaces on Tetracene and Pentacene Thin-Films via Monolayers

Selma Piranej,^a David A. Turner,^a Shawn M. Dalke,^a Haejun Park,^a Brittini A. Qualizza,^a Juvinch Vicente,^b Jixin Chen,^b Jacob W. Ciszek^{*a}

Address

^a Department of Chemistry and Biochemistry, Loyola University Chicago,
Chicago, Illinois 60660, USA, Email: jciszek@luc.edu,

^b Department of Chemistry and Biochemistry, Ohio University, Athens, Ohio 45701, USA

Table of Contents

IR Spectra of Organic Compounds and Substrates

ATR-IR spectrum of the standard <i>N</i> -methylmaleimide	...2
ATR-IR of standard tetracene	...2
ATR-IR of the standard tetracene- <i>N</i> -methylmaleimide adduct	...3
ATR-IR of a 10:1 mole ratio of tetracene to the standard tetracene- <i>N</i> -methylmaleimide adduct	...3

Additional Regions of Interest from Tetracene Reacted Surfaces

Tetracene film reacted with <i>N</i> -methylmaleimide 1225-1075 cm ⁻¹	...4
Tetracene film reacted with <i>N</i> -methylmaleimide 1350-1200 cm ⁻¹	...4

IR Spectrum for Sublimed *N*-methylmaleimide

<i>N</i> -methylmaleimide sublimed onto a tetracene thin film	...5
---	------

AFM data

Unreacted and reacted tetracene films5
---------------------------------------	-------

Additional Regions of Interest from Tetracene Reacted Surfaces

Pentacene film reacted with <i>N</i> -methylmaleimide 1200-1050 cm ⁻¹	...6
--	------

Contact Angle Data	...6-7
---------------------------	--------

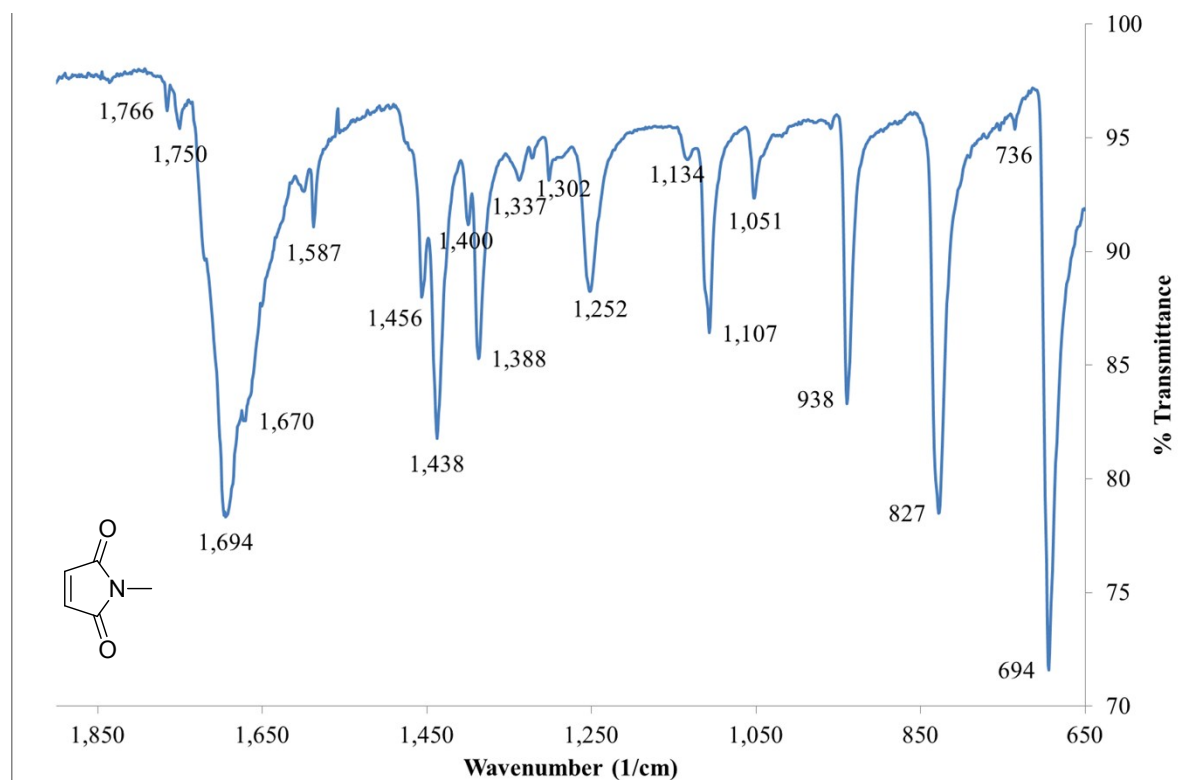


Fig. S1: An ATR-IR spectrum of the standard N-methylmaleimide from 1900-650 cm^{-1} .

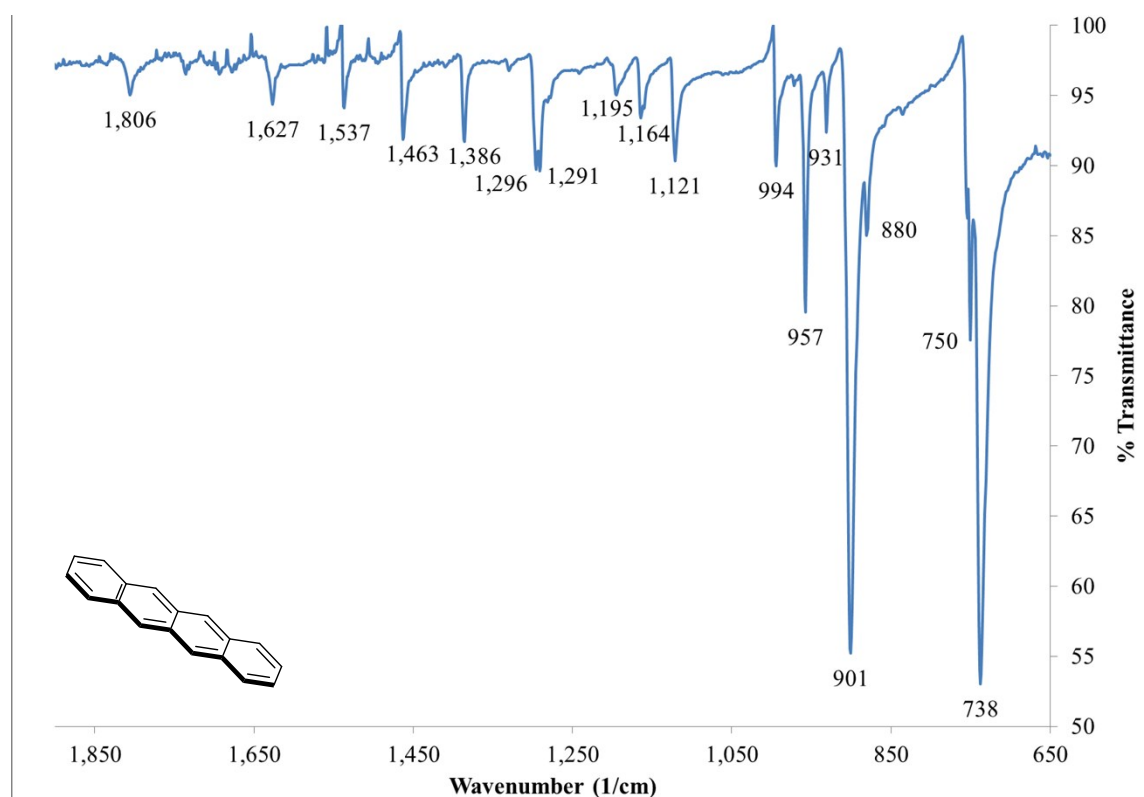


Fig. S2: An ATR-IR of standard tetracene from 1900-650 cm^{-1} .

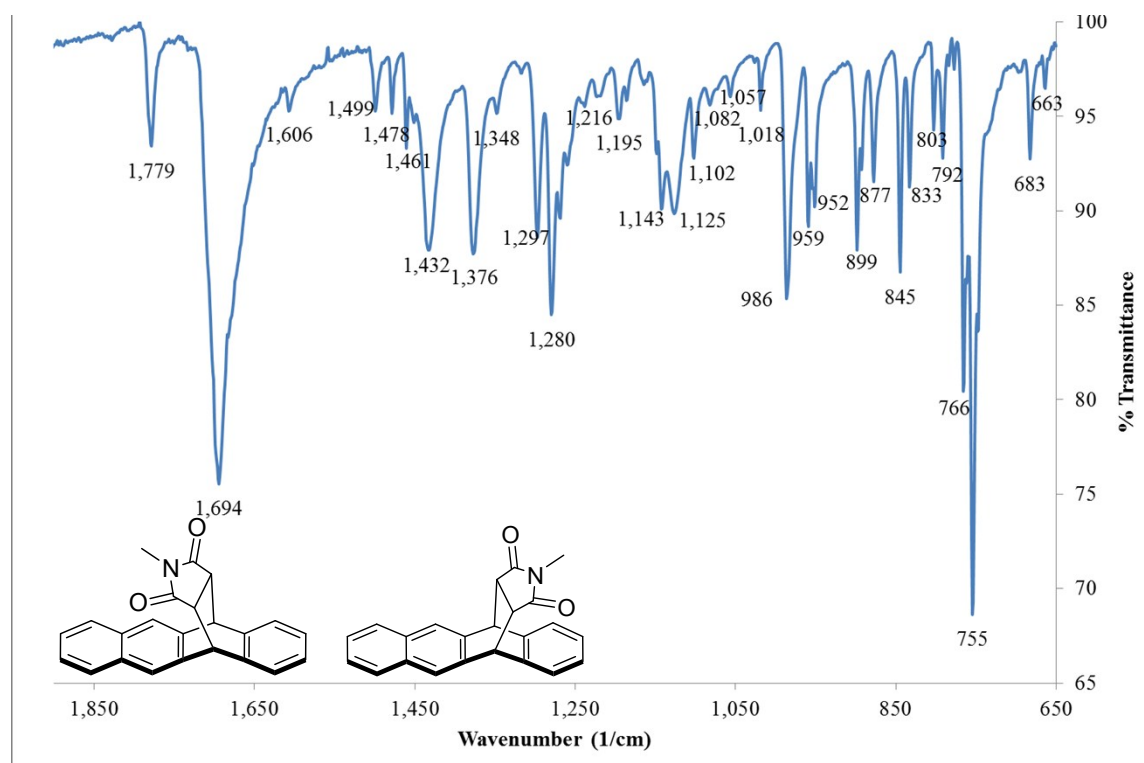


Fig. S3: An ATR-IR of the standard tetracene-*N*-methylmaleimide adduct from 1900-650 cm^{-1} .

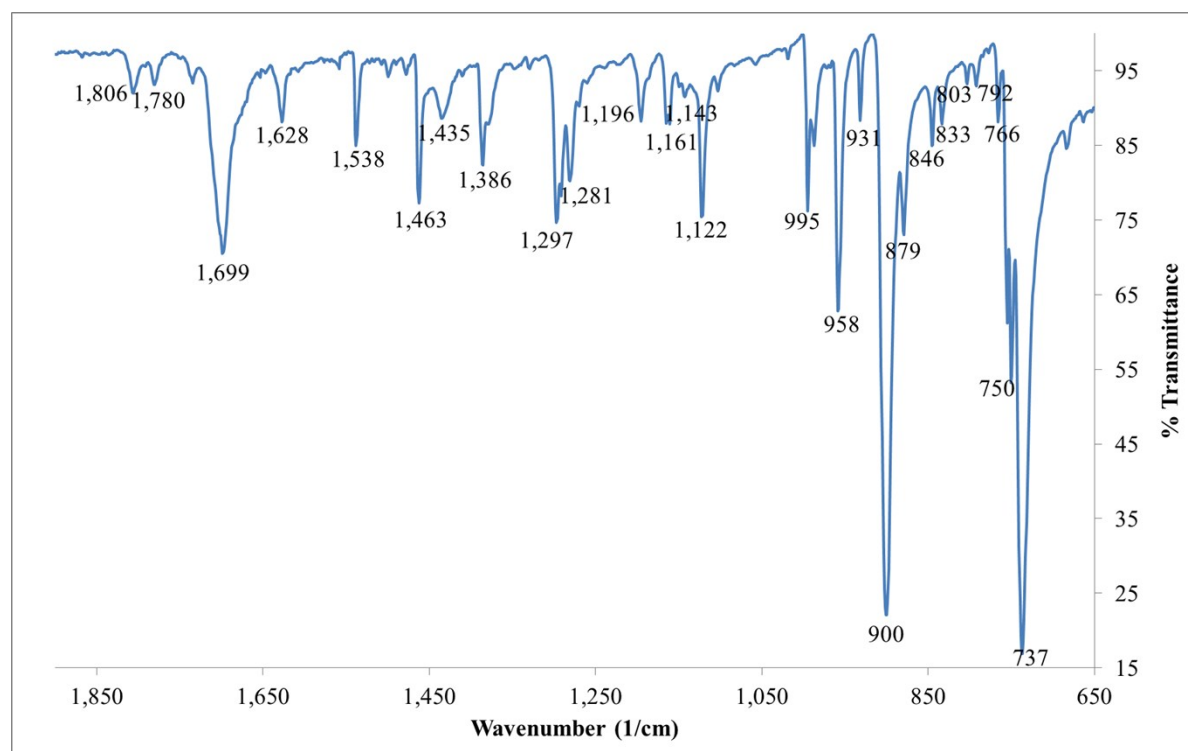


Fig. S4: An ATR-IR of a 10:1 mole ratio of tetracene to the standard tetracene-*N*-methylmaleimide adduct.

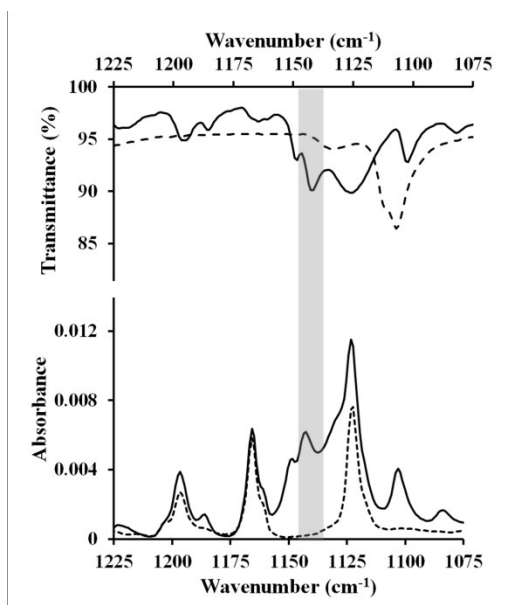


Fig. S5: A comparison of a PMIRRAS-IR spectrum of a film of tetracene that was exposed to N-methylmaleimide (below) with the standard powder adduct taken via ATR-IR (above). The ATR-IR spectrum shows that N-methylmaleimide (dashed line) has little absorption above 1100 cm^{-1} allowing this region to be used for observing formation of the standard Diels- Alder adduct (solid line, above and below). The diagnostic peak at 1143 cm^{-1} is observed in the reacted substrate (solid line, bottom), and is not present in the pristine thin film (dashed line).

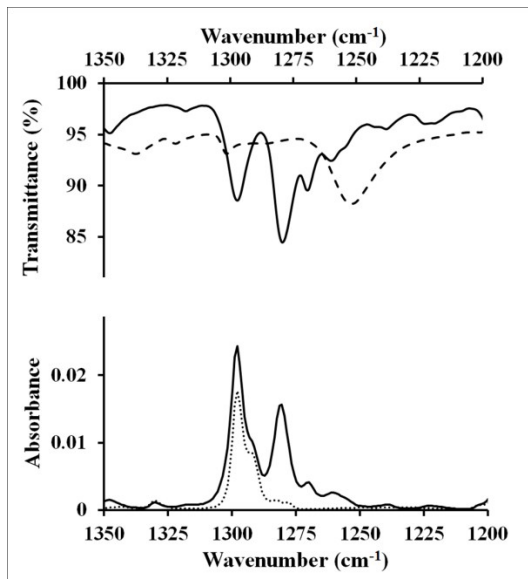


Fig. S6: A comparison of a PMIRRAS-IR spectrum of a film of tetracene that was exposed to N-methylmaleimide (below) with the standard powder adduct taken via ATR-IR (above). The PMIRRAS-IR spectrum shows tetracene (dotted line) and the Diels-Alder adduct film (solid line) and the appearance of a peak at 1280 cm^{-1} . The ATR-IR spectrum displays N-methylmaleimide (dashed line) and the standard Diels-Alder adduct (solid line). The peak at 1280 cm^{-1} indicates formation of the Diels-Alder adduct.

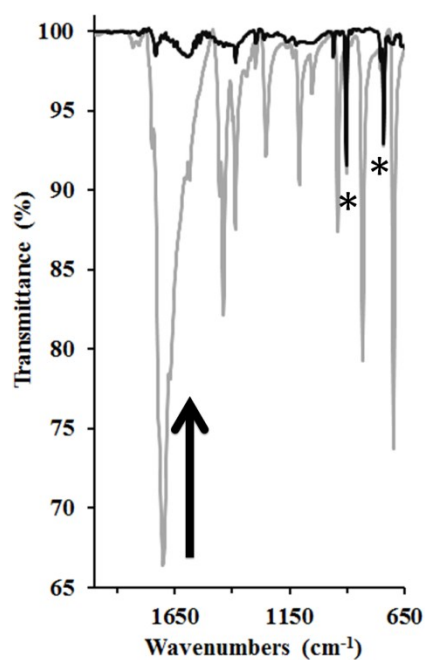


Fig. S7: Light gray line is a tetracene thin-film on a salt plate with N-methylmaleimide sublimed on top. After 5 min exposure to a gentle stream of nitrogen (black line) the N-methylmaleimide features (e.g. 1705 cm^{-1} , arrow) disappear, leaving only vibrations from the tetracene thin film (starred).

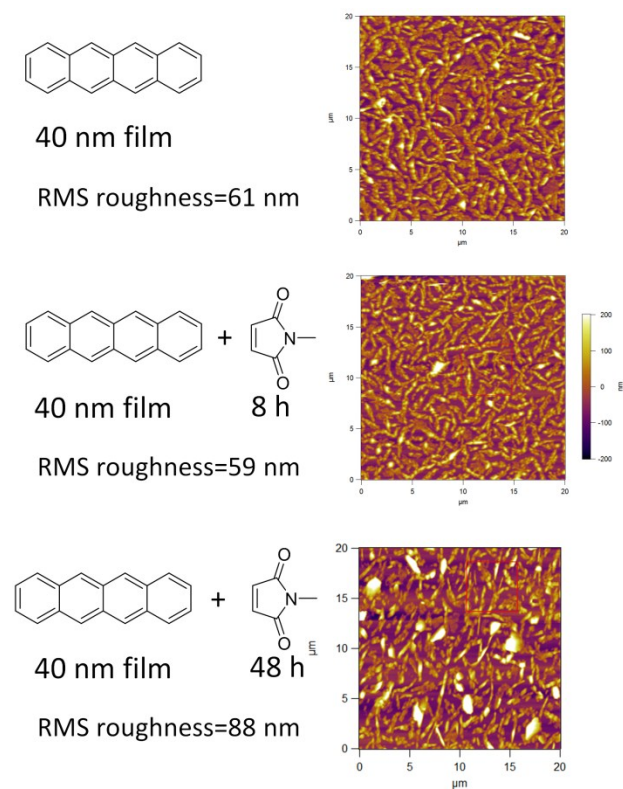


Fig. S8: AFM data of unreacted and reacted tetracene films. RMS data is for the scanned window.

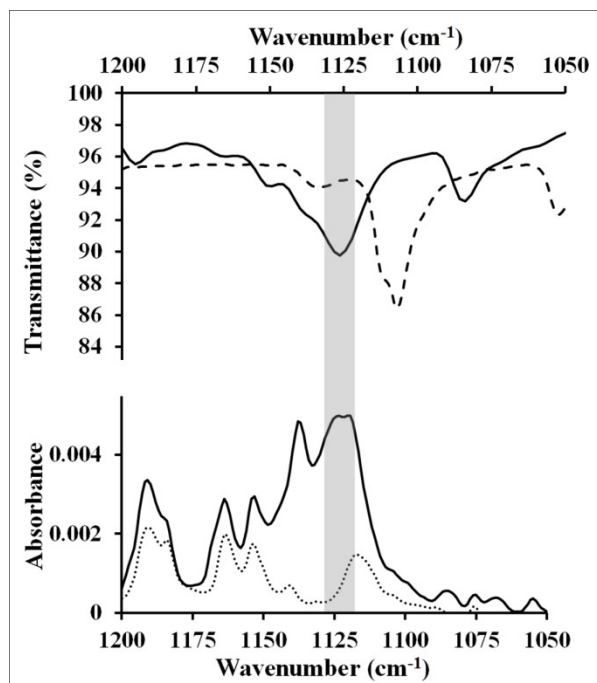


Fig. S9: A comparison of a PMIRRAS-IR spectrum of a film of pentacene that was exposed to N-methylmaleimide (below) with the standard powder adduct taken via ATR-IR (above). The PMIRRAS-IR spectrum shows tetracene (dotted line) and the Diels-Alder adduct film (solid line) and the appearance of a peak at 1126 cm^{-1} . The ATR-IR spectrum displays N-methylmaleimide (dashed line) and the standard Diels-Alder adduct (solid line). The diagnostic peak at 1126 cm^{-1} indicates formation of the Diels-Alder adduct.

Contact Angle Data

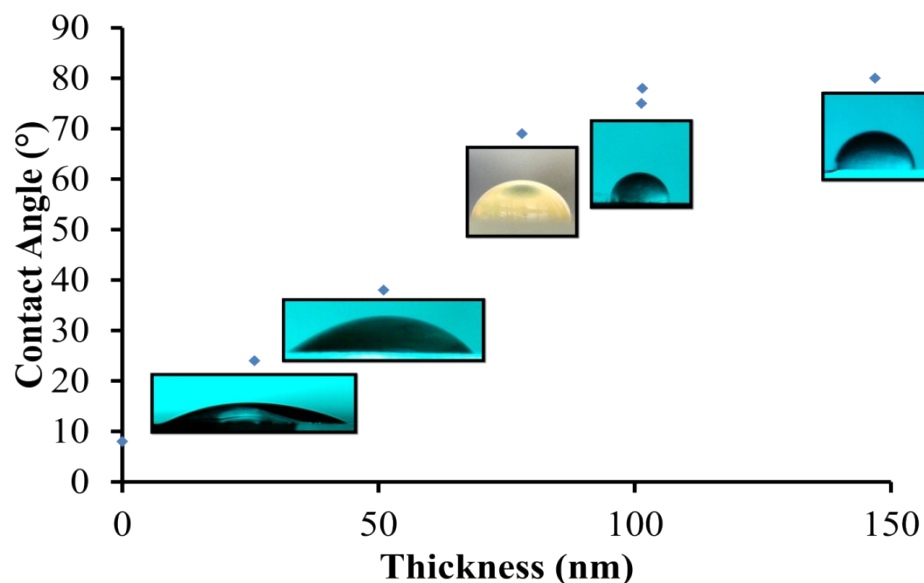


Fig. S10: A graph of contact angle ($^{\circ}$) versus thickness (nm) of tetracene used to determine the baseline contact angle.

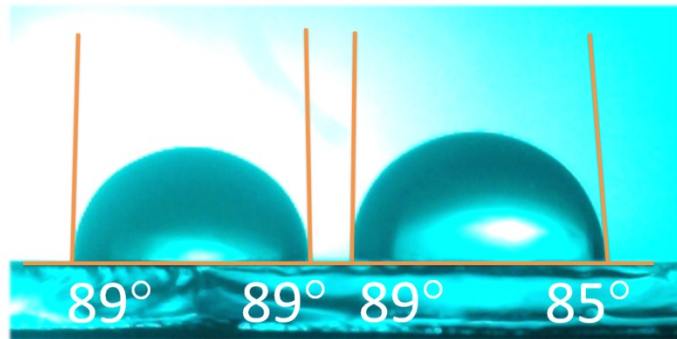


Fig. S11: Contact angle measurement on a 100 nm tetracene surface after exposure to water vapor for 48h.