Raman spectra calculation for single molecule Observed by Tip-Enhanced Raman Spectroscopy

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Purpose: This study demonstrates a tip-enhanced Raman spectroscopy (TERS)-induced chemical reaction by immobilizing molecules with a self-assembled monolayer on a Au(111) surface. The Raman spectrum of an isolated molecule and their derivatives were calculated to compare with the TERS spectrum.

Substance: The intensities of the Raman spectra were converted from the calculated Raman activities using an equation which is available in the Chemcraft software. Raman spectra of an isolated pristine [7]TH-aldehyde molecule, and of the isolated [7]TH-aldehyde molecule with the *L*-mode localized at the side (L_1), center (L_2) and on all three benzene rings (L_3) were calculated..

Results: According to the calculated spectra, the L_1- and L_2-modes result in peaks at 1996 and 2012 cm^{-1}, respectively. By the comparison to the experimental results, it is deduced that one side benzene ring which protruded upwards close to the tip had undergone hydrogenation induced by pyrolysis with the tip acting as both local heat source and catalyst.

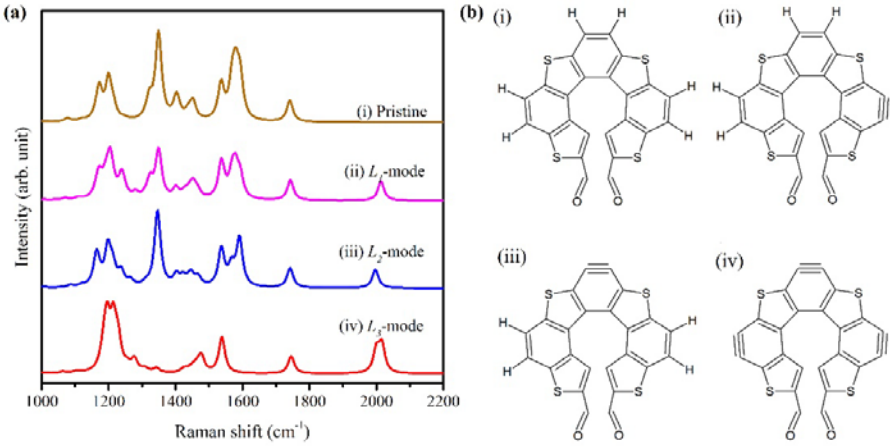

Fig. 1. (a) Calculated Raman spectra and (b) molecular structure of pristine (i), L_1-mode (ii), L_2-mode (iii), and L_3-mode (iv) of [7]TH-aldehyde.

Machine	VCC
Used Nod	2000hour
Memory	470GB