

Vibrational spectra and surface-enhanced vibrational spectra of 1-nitropyrene

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The present report on the vibrational spectra of 1-nitropyrene (1-NP) describes the infrared and Raman spectra; their interpretation is aided by local density functional theory (DFT) calculations at the B3LYP/6-311G(d,p) level of theory and by the surface-enhanced vibrational spectra (SEVS) with the final objective of trace organic analytical applications. The surface-enhanced Raman scattering (SERS) on silver island films and mixed silver/gold island films was investigated with several laser lines in the visible region. Surface-enhanced infrared absorption (SEIRA) was attempted on silver and gold island films. The interface of the organic 1-NP with smooth metal surfaces of silver and copper was also probed using reflection-absorption infrared (RAIRS) spectra that, in conjunction with the transmission spectra, allow one to extract the molecular orientation in vacuum evaporated thin solid films. Chemical adsorption of 1-NP on silver and further photochemical decomposition of the 1-NP-me