MICROWAVE SPECTRA AND GEOMETRIES OF C₂H₂ ⋯ AuI and C₂H₄ ⋯ AuI

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A chirped-pulse Fourier transform microwave spectrometer has been used to measure the microwave spectra of both C₂H₂ ⋯ AuI and C₂H₄ ⋯ AuI. These complexes are generated via laser ablation at 532 nm of a gold surface in the presence of CF₃I and either C₂H₂ or C₂H₄ and argon and are stabilized by a supersonic expansion. Rotational (A₀, B₀, C₀) and centrifugal distortion constants (ΔJ, ΔJK and δJ) of each molecule have been determined as well the nuclear electric quadrupole coupling constants of gold and iodine atoms (χₐₐ (Au), χₜₜ (Au), χₙₙ (I) and χₜₜ − χₙₙ (I)). The spectrum of each molecule is consistent with a C₂v structure in which the metal atom interacts with the π-orbital of the ethene or ethyne molecule. Isotopic substitutions of atoms within the C₂H₂ or C₂H₄ subunits are in progress and in conjunction with high level ab initio calculations will allow for accurate determination of the geometry of each molecule.