

MICROWAVE SPECTRA AND GEOMETRIES OF $C_2H_2 \cdots AgI$ and $C_2H_4 \cdots AgI$

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A chirped-pulse Fourier transform microwave spectrometer has been used to measure the microwave spectra of both $C_2H_2 \cdots AgI$ and $C_2H_4 \cdots AgI$. These complexes are generated via laser ablation at 532 nm of a silver surface in the presence of CF_3I and either C_2H_2 or C_2H_4 and argon and are stabilized by a supersonic expansion. Rotational (A_0 , B_0 , C_0) and centrifugal distortion constants (Δ_J and Δ_{JK}) of each molecule have been determined as well the nuclear electric quadrupole coupling constants the iodine atom ($\chi_{aa}(I)$ and $\chi_{bb} - \chi_{cc}(I)$). The spectrum of each molecule is consistent with a C_{2v} structure in which the metal atom interacts with the π -orbital of the ethene or ethyne molecule. Isotopic substitutions of atoms within the C_2H_2 or C_2H_4 subunits are in progress and in conjunction with high level *ab initio* calculations will allow for accurate determination of the geometry of each molecule. These two complexes are put in the context of the recently studied $H_2S \cdots AgI$,^a $OC \cdots AgI$,^b $H_3N \cdots AgI$ and $(CH_3)_3N \cdots AgI$.^c

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^cD.M. Bittner, D.P. Zaleski, S.L. Stephens, N.R. Walker, A.C. Legon, Study in progress.