MICROWAVE SPECTRA AND STRUCTURES OF $H_4C_2\cdots AgCl$ AND $H_4C_2\cdots CuCl$

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A Balle-Flygare FT-MW spectrometer coupled to a laser ablation source has been used to measure the pure rotational spectra of $H_4C_2\cdots AgCl$ and $H_4C_2\cdots CuCl$. Both molecules are generated via laser ablation (532 nm) of a metal rod in the presence of CCl_4, C_2H_4 and argon and are stabilized by supersonic expansion. Rotational constants (A_0, B_0, C_0) and the centrifugal distortion constant, D_J, have been measured for six isotopologues of $H_4C_2\cdots AgCl$ and five isotopologues of $H_4C_2\cdots CuCl$ with substitutions at the metal, chlorine and carbon atoms in each case. The spectrum of each molecule is consistent with a C_{2v} structure in which the metal atom interacts with the π-orbital on ethene. The measured rotational constants allow determination of the length of the bond between the metal and chlorine atoms, r_{MCl}, and the distance between the metal atom and the centre of the ethene double bond, r_{MEt}. Nuclear quadrupole coupling constants have been determined for the chlorine atom in each molecule and also for copper in $H_4C_2\cdots CuCl$.