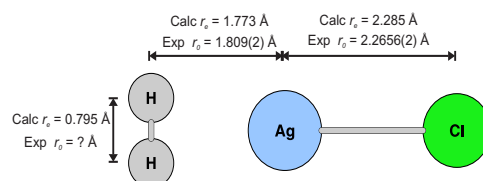


FTMW OBSERVATION AND ANALYSIS OF THE *p*-H₂-AgCl AND *o*-H₂-AgCl COMPLEX

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The rotational spectrum of *p*-H₂-AgCl and *o*-H₂-AgCl has been measured for the first time using a Balle-Flygare type Fourier transform microwave (FTMW) spectrometer. $\frac{(B+C)}{2}$'s, nuclear quadrupole coupling constants, and centrifugal distortion constants have been determined for multiple isotopologues of both species while spin-spin coupling constants have also been determined for at least one isotopologue of the *o*-H₂ species. Substantial changes in the eQq value from the monomer^a occur at the Cl nucleus upon complexation with the H₂ and will be discussed. Experimental r_0 's for the H₂ C.O.M. distance to Ag and Ag distance to Cl are 1.809(2)Å and 2.2656(2)Å, respectively, for the *p*-H₂ species and will be compared to theory. Quantum chemical calculations were performed with an APFD^b density functional and MP2 with an aug-cc-pVQZ basis set for the hydrogen and chlorine with the effective core potential ECP28MDF_AVQZ^{c,d} for the Ag and will be presented.



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