FTMW OBSERVATION AND ANALYSIS OF THE p-H_2–AgCl AND o-H_2–AgCl COMPLEX

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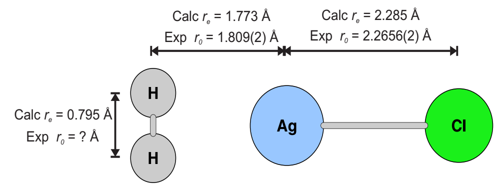

The rotational spectrum of p-H_2–AgCl and o-H_2–AgCl has been measured for the first time using a Balle-Flygare type Fourier transform microwave (FTMW) spectrometer. $\frac{(B+C)}{2}$'s, nuclear quadrupole coupling constants, and centrifugal distortion constants have been determined for multiple isotopologues of both species while spin-spin coupling constants have also been determined for at least one isotopologue of the o-H_2 species. Substantial changes in the eQq value from the monomer[a] occur at the Cl nucleus upon complexation with the H_2 and will be discussed. Experimental r_0's for the H_2 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-H_2 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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