FTMW OBSERVATION AND ANALYSIS OF THE $p$–H$_2$–AgCl AND $o$–H$_2$–AgCl COMPLEX

G. S. GRUBBS II, DANIEL A. OBENCHAIN, HERBERT M. PICKETT and STEWART E. NOVICK, Department of Chemistry, Wesleyan University, 52 Lawn Avenue, Middletown, CT, 06459-0180, USA (email to GSG2: ggrubbs@wesleyan.edu).

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. The 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 $\varepsilon Qq$ value from the monomer 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\textsuperscript{b} density functional and MP2 with an aug-cc-pVQZ basis set for the hydrogen and chlorine with the effective core potential ECP28MDF\textsuperscript{c,d} for the Ag and will be presented.