HYDROGEN INTERACTION WITH METAL HALIDES: THE NUCLEAR QUADRUPOLE COUPLING CONSTANT OF GOLD IN THE p-H_2-AuCl COMPLEX AND TRENDS IN THE OTHER HYDROGEN-COINAGE METAL HALIDE INTERACTIONS

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The rotational spectrum of p-H_2-AuCl has been measured using a laser ablation equipped FTMW cavity spectrometer. The predicted structure, using a 60 electron core potential and an aug-cc-pVQZ[ab] at the MP2 level of theory, shows that H_2 has an $r_e = 0.91$Å. A predicted value for the $eQq(\chi_{aa})$ of gold required a semi-empirical method using the results of previous AuCl complexes in the gas phase. Transitions have been measured across multiple J levels, and have been used to determine the rotational constants, centrifugal distortion constants, and nuclear quadrupole coupling constants of multiple isotopologues. The o-H_2-AuCl has also been observed. While the monomer value of the *eQq* of ^{197}Au was determined to be 9.63112(13) MHz in $^{197}Au^{35}Cl$[c], we observed a significant change in the *eQq* of ^{197}Au in p-H_2-$^{197}Au^{35}Cl$ to a value of -817.9983(36) MHz [0.02728556(12) cm^{-1}], giving rise to a Au hyperfine component splittings of approximately 220 MHz [0.007 cm^{-1}] and suggesting a change in electronic structure with the interaction of H_2. We will present a summary of the hydrogen-coinage metal halide talks given at this conference, including trends in *eQq* and hydrogen metal halide dissociation energies.

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