OBSERVATION OF A MODERATE STRENGTH INTERACTION OF HYDROGEN WITH A COINAGE METAL HALIDE: THE ROTATIONAL SPECTRUM AND STRUCTURE OF THE p-H_2-CuCl AND o-H_2-CuCl COMPLEXES

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Rotational transitions of the p-H_2-CuCl and o-H_2-CuCl have been observed on a laser ablation equipped FTMW cavity instrument. Computational studies preformed using the APFD[a] density functional and MP2 level of theory were used to predict the structure of the p-H_2-CuCl. Measurements from the J=1–0 to the J=3–2 transitions were used to determine the rotational constants, centrifugal distortion constants, and quadrupole coupling constants for multiple isotopologues of the p-H_2-CuCl species. Similar constants, including spin-spin coupling constants, have also been determined for the o-H_2-CuCl species for the J=2–1 and the J=3–2 transitions. The eQq of the copper in p-H_2-$^{63}Cu^{35}Cl$ was found to be 52.058(2) MHz, a change from the monomer $^{63}Cu^{35}Cl$ value of 16.1712(24) MHz[b].

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