THE COMBINED ORTHO / PARA HYDROGEN ASSIGNMENTS IN H2 METAL CHLORIDES

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The rotational spectra of H_2 -AgCl and H_2 -AuCl have been measured using a cavity FTMW spectrometer equipped with a laser ablation source. A combination of isotopic substitution, including HD and D_2 substitutions, and the spin-spin interaction of *ortho* hydrogen were used to determine the structures of these species. Trends in these structures and the strengths of the H_2 interaction will be discussed.

Previous work with hydrogen containing complexes have shown that separate spectra are observed for the both the *ortho* and *para* hydrogen species. a;b;c In this work, *ortho* and *para* hydrogen are assigned together. The a-axis in the present species is coincident with internal rotation axis of hydrogen. This symmetry, along with a covalent interaction of the H_2 with the metal chlorides, allows for a straightforward global assignment of the *ortho* and *para* species. The differences in the present study from the previous works will be discussed, as well as the assignment of the combined *ortho* and *para* fits.

^aY. Zhenhong, K. J. Higgins, W. Klemperer, M. C. McCarthy and P. Thaddeus, J. Chem. Phys., 123(2005) 221106.

^bJ. M. Michaug, W. C. Topic, W. Jäger, J. Phys. Chem. A., **115**(2011) 9456.

^cM. Ishiguro, K Harada, K. Tanaka, Y. Sumiyoshi, Y. Endo, *Chem. Phys. Lett.*, **554**(2012) 33.