VIBRATIONAL AND HYPERFINE COUPLING EFFECTS IN $(HI)_2$

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The rotational-vibrational microwave transitions of HI dimer, consisting of a-type $K_a = 0 \leftarrow 0$ transitions between the two lowest vibrational states of the dimer, were reported in a previous presentation.[a] In a preliminary analysis, the frequencies of these transitions were fitted using a vibrational frequency and, for each vibrational state, B and D_J constants and an effective quadrupole coupling constant χ_{aa}. The value of the root mean square deviation, 85 kHz, was more than 50 times larger than the experimental uncertainty on the transition frequencies.

In this presentation the submillimeter data of HI dimer is reinvestigated using a theoretical model accounting for the interaction between the dimer geared-type vibrational motion and the quadrupole coupling arising from each HI subunit. As in the approach developed for the ethylene diamine molecule,[b] the present formalism accounts for the fact that the rovibrational part of the matrix elements of the hyperfine coupling Hamiltonian is strongly dependent on whether these matrix elements are calculated within or between vibrational states. Such effects, which were ignored in the preliminary analysis, are very important because of the very large value of the eqQ quadrupole coupling constant of an HI molecule.[c]

The theoretical model allows us to reproduce the 345 available transitions with a root mean square deviation on the order of 18 kHz. In the presentation, these results will be presented and we will try to see if they can be further improved. Values for the various components of the effective quadrupole coupling tensors obtained from the analysis will be compared to those retrieved using *ab initio* calculations.

[a] McElmurry, Lucchese and Bevan, Paper RB08, 60th International Symposium on Molecular Spectroscopy, Columbus, Ohio, USA, June 20–24, 2005

[b] Merke and Coudert, *J. Molec. Spectrosc.* **237,** 174 (2006).

[c] Chance, Varberg, Park, and Zink, *J. Molec. Spectrosc.* **162,** 120 (1993).