LARGE AMPLITUDE MOTIONS EFFECTS IN THE HYPERFINE STRUCTURE OF THE CD_4–D_2O COMPLEX

Y. KAWASHIMA, *Department of Applied Chemistry, Kanagawa Institute of Technology, 1030 Shimo-ogino, Atsugi, Kanagawa 243-0292, Japan*; AND L. H. COUDERT, *Laboratoire de Photophysique Moléculaire, C.N.R.S., Bât. 350, Université Paris-Sud, 91405 Orsay Cedex, France*.

The CD_4–D_2O complex is an interesting molecular species displaying a fairly complicated hyperfine structure arising from quadrupole coupling of the six deuterium atoms. Just like its normal species CH_4–H_2O[a] and its partially deuterated species CD_4–H_2O,[b] this complex is also a very non-rigid one in which each subunit undergoes nearly free internal rotation.

New measurements of the rotational spectrum of the CD_4–D_2O complex have been carried out at Kanagawa Institute of Technology using a Fourier transform microwave spectrometer. The data set involves $J = 1 \leftarrow 0$ and $J = 2 \leftarrow 1$ rotational transitions displaying a hyperfine structure which could be experimentally resolved. Based on these hyperfine patterns and on the transitions intensities, it was possible to label the observed internal rotation levels with the $E^{\pm}$, $F^{\pm}$, and $A^{\pm}$ symmetry species of G_{48}, for increasing frequencies. This ordering turned out to be different to that found[a] in CH_4–H_2O which was F, E, and A. Also the splitting between $\pm$ states was found larger than in CD_4–H_2O[b] and this is attributed to larger asymmetry effects.

It is the goal of the present investigation to analyze the observed hyperfine patterns in order to obtain quantitative information on the intramolecular potential of the complex. Starting from the intramolecular potential introduced in the case of the normal species,[a] the rovibrational wavefunctions of the complex will be obtained[c] for all symmetry species. These wavefunctions will be afterwards used to evaluate matrix elements of the hyperfine Hamiltonian and to calculate the hyperfine structure of the measured transitions. At last, by matching observed and calculated hyperfine patterns, we hope to obtain values for the spectroscopic parameters characterizing the intramolecular potential of the complex.

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[a] Dore, Cohen, Schmuttnmaer, Busarow, Elrod, Loeser, and Saykally, *J. Chem. Phys.* **100,** 863 (1994) and Suenram, Fraser, Lovas, and Kawashima, *J. Chem. Phys.* **101,** 7230 (1994).

[b] Kawashima and Coudert, 57th International Symposium on Molecular Spectroscopy, paper **TI08** (2002).

[c] Brocks, van der Avoird, Sutcliffe, and Tennyson, *Molecular Physics* **50,** 1025 (1983).