Millimeter wave spectroscopy of CH_3ReO_3

T. R. Huet [a], L. Margulès [a], and R. Motiyenko [a]

[a] Laboratoire PhLAM, CNRS-Université Lille 1, F-59655 Villeneuve d'Ascq Cedex, France ;
E-mail: Therese.Huet@univ-lille1.fr

Originating from the weak interaction, parity violation in chiral molecules has been considered as a possible origin of biohomochirality. The Chardonnet's group at LPL proposed the observation of molecular parity violation using the two-photon Ramsey fringes technique on a supersonic beam. As a first step in this direction, a detailed spectroscopic study of methyltrioxorhenium (MTO) was undertaken. It is an ideal test molecule as the achiral parent molecule of chiral candidates for a parity violation experiment. For the ^{187}Re MTO isotopologue, a combined analysis of Fourier transform microwave [1, 2] and infrared spectra as well as ultra-high resolution CO_2 laser absorption spectra enabled the assignment of 28 rotational lines and 71 rovibrational lines, some of them with a resolved hyperfine structure. A set of spectroscopic parameters in the ground and first excited state, including hyperfine structure constants, was obtained for the ν_{as} antisymmetric Re=CO stretching mode of this molecule. This result validated the experimental approach to be followed once a chiral derivative of MTO is synthesized, and showed the benefit of the combination of several spectroscopic techniques in different spectral regions, with different set-ups and resolutions [2].

In the present work we have extended the rotational analysis of the MTO spectrum in the millimeter wave region. The spectra were recorded at room temperature, with the residual vapor pressure, in the 150-300 GHz range. The rotational and hyperfine structure of $CH_3{}^{185}ReO_3$ and $CH_3{}^{185}ReO_3$ was characterized up to J, K = 42/42 in the ground state. More than 900 lines have been assigned for each isotopolog, and a new set of parameters has been obtained, which namely includes a rotational correction to the quadrupolar hyperfine constant. This new set of parameters characterizes – for the ground state - the whole set of quantum numbers observed in the IR spectra and should allow a refined IR analysis, for both isotopologs.

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