HIGH RESOLUTION ASSIGNMENT OF ν_{14} AND ν_{16} BANDS IN THE 10 μM FOR TRANS-ACROLEIN

XINGJIE JIANG, LI-HONG XU, *Centre for Laser, Atomic and Molecular Sciences (CLAMS), Dept. of Physical Sciences, Univ. of New Brunswick, Canada E2L 4L5*; A.R.W. MCKELLAR, *Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, Canada*.

Acrolein (CH_2CHCHO) is one of the four (in addition to methanol CH_3OH, acetaldehyde CH_3CHO, and 1,3-butadiene $CH_2CHCHCH_2$) 2004 target molecules from main- and side-stream (MS and SS) cigarette smoke[1]. The present work is aimed at extending the database of high resolution laboratory spectroscopic information on the molecule in the 10 μm region.

We have obtained 10 μm high resolution spectra from NRC both at room and cooled temperatures at 0.002 cm^{-1} resolution. The spectra cover several vibrational bands including the two dominant ones, the ν_{16} CH_2 out-of-plane rocking and ν_{14} CH2 twisting. Analyses of the ν_{16} and ν_{14} bands are now at advanced stages. More specifically, about 1085 lines have been assigned to the ν_{16} band for transitions to upper state Ka' = 0, 1, 2, 3, 4, 5, 6, 7, 8, 9 and 10, and about 800 lines have been assigned to the ν_{14} band for transitions to upper state Ka' = 1, 2, 3, 4, 5, 6, 7 and 8. We have applied an isolated band model to each band using Maki's asymmetric rotor Hamiltonian in which some assigned transitions were removed from our fits. In our analysis, we have encountered challenges due to high line density as well as perturbations. For the latter, J-reduced upper state term values have been obtained and plotted as a function of J, indicating possible interactions among the two states.

For intensity information, we have carried out $ab\,initio$ dipole derivative calculations using the procedure explained in Ref. [2] for 1,3-butadiene. A line list with position and intensity has been compiled using the $ab\,initio$ dipole derivatives and the rotational constants obtained from the present work.

[1] Private communication from Aerodyne Research, Inc., and Phillip Morris Research Center.

[2] Z.D. Sun, Li-Hong Xu, R.M. Lees, X.J. Jiang, S. Perry, N.C. Craig, J. Mol. Struct. 742 (2005) 69-76.