LAMB-DIP OBSERVATIONS OF COMPACT Q-BRANCHES IN THE 11 μm REGION FOR 1,3 BUTADIENE

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The CH_2-wagging vibrational mode of 1,3 butadiene centred at 908 cm^{-1} or 11 μm is a well defined c-type band. The Fourier transform spectrum of this band was recently recorded at 0.00184 cm^{-1} resolution in the Giessen laboratory. Apart from some unresolved Q-branch heads for medium to high-K Q-branches, analysis is at an advanced stage with energy levels observed up to K_{max} of about 10 and J_{max} near 70 for unperturbed infrared transitions. With 9 parameters (V_o, A, B, C, d_J, d_K, D_J, D_{JK}, D_K), assignments have been fit to a Watson-type asymmetric rotor Hamiltonian in A-reduction to experimental accuracy (1).

We have recently carried out Lamb-dip measurements for some unresolved Q-branch heads. Our motivations are (i) to test the performance of our newly built CO_2-laser/microwave sideband spectrometer in the 11 μm region, (ii) to resolve these overlapped features in the FTS (Doppler limited) with sub-Doppler technique (Lamb-dip) in order to provide accurate line positions and assignments for these components, and (iii) to obtain an estimate of the transition dipole moment for this band. The latter is an important piece of information needed for possible cigarette smoke detection with a tunable diode laser system (2). Under broad band scanning mode at Doppler limited resolution, we have observed K = 10 $\leftarrow$ 9, 9 $\leftarrow$ 8, 8 $\leftarrow$ 7, 7 $\leftarrow$ 6, 6 $\leftarrow$ 5, and 5 $\leftarrow$ 4 Q-branch heads. They are strong features in the spectrum. In order to resolve these heads, sub-Doppler Lamb-dip experiments were performed. So far, we have resolved K = 9 $\leftarrow$ 8, 8 $\leftarrow$ 7, and 7 $\leftarrow$ 6 Q-branch heads with the Lamb-dip technique. Our fully resolved components are consistent with line predictions based on a previous FT analysis (1). From comparison of the weakest Lamb-dip signals observed in our experiment for this molecule with those of other molecules (such as CH_3OH and OCS), we have deduced a very rough estimate of about 0.5 Debye $\Delta\mu_c$ transition dipole moment for this band. Work is in progress for sub-Doppler observations of other K value Q-branch heads.

(1) N.C. Craig, J.L. Davis, K.A. Hanson, M.C. Moore, K.J. Weidenbaum, M. Lock, J. Mol. Struct., 2004, in press.

(2) Q. Shi, D.D. Nelson, J.B. McManus, M.S. Zahniser, C.N. Harward, Anal. Chem. 75, 5180-5190 (2003).