RADIO FREQUENCY-INFRARED DOUBLE RESONANCE MEASUREMENT OF THE ELECTRIC DIPOLE MOMENT IN BEND-STRETCH COMBINATION VIBRATIONAL STATES OF HCCD

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With a small permanent electric dipole moment due to differences in zero point motion between hydrogen and deuterium, monodeuteroacetylene, HCCD, is particularly well-suited for studying changes in the dipole moment upon vibrational excitation. In fact, for several normal modes, the change in dipole moment accompanying excitation of one quantum of vibration is larger than the ground state moment. We have used radio frequency-infrared double resonance to directly measure the Stark shift of the $J = 1$ ℓ-doublet splitting in four vibrational states of HCCD. New results were obtained for two C-H stretch plus bend combination states. For the combination with the C-D bend, $\nu_1 + \nu_4$, $q_\ell = 132.289(6)$ MHz and $\mu = 0.046627(33)$ D, while for the combination with the C-H bend, $\nu_1 + \nu_5$, $q_\ell = 107.263(4)$ MHz and $\mu = 0.031385(22)$ D. Our measurements on the two bending fundamentals, ν_4 and ν_5, were combined with earlier molecular beam electric resonance [a] and microwave [b] results to provide electric field calibration. Additionally, it appears that infrared spectra involving the $\nu_1 + \nu_4$ state have not previously been reported. Our data allow us to provide preliminary measurements for the rotational constant in this state and for the band origin of the $\nu_1 + \nu_4 - \nu_4$ hot band, namely $B = 0.9892$ cm^{-1} and $\nu_0 = 3331.46$ cm^{-1}.

[a] M. D. Marshall, and W. Klemperer, J. Chem. Phys. 81, 2928 (1984).
[b] K. Matsumura, T. Tanaka, Y. Endo, S. Saito, and E. Hirota, J. Phys. Chem. 84, 1793 (1980).