FIRST HIGH RESOLUTION IR SPECTRA OF 2-D₁-PROPANE. THE $\nu_9$ ($A_1$) B-TYPE BAND NEAR 367.2389 cm$^{-1}$.

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This is a further report in a project to record high resolution IR data of the $^{13}$C and D substituted isotopologues of propane (see talks FA04, FA05 and TK08 at 2017 ISMS). Initially in CLS Cycle 23 (Jan-Jun, 2015) we recorded spectra of the $\nu_{26}$ ($B_2$) C-Type band whose corresponding band in $C_3H_8$ is observed in Titan’s Atmosphere. That band and others seen in the 550-950 cm$^{-1}$ region were too perturbed by complex torsional splittings for analysis at this time. In this talk will give details on the first high resolution ($\Delta \nu = 0.00096$ cm$^{-1}$) IR investigation of the spectrum in the Far-IR region. We recorded spectra during Cycle 25 (Jan-Jun, 2017) of the $\nu_9$ ($A_1$) CCC skeletal bending mode near 367.2389 cm$^{-1}$. This has a B-type band structure and appears unperturbed. Spectra were recorded at pressures of 0.014, 0.056, 3.995 & 8.087 Torr in a 72m optical path at room temperature. We used the Bruker IFS-125HR on the Far-IR beamline of the CLS. The spectra were assigned both traditionally and with the aid of the PGOPHER program of Colin Western. We were able to assign over 8100 lines with up to $K = 35$ and $J = 60$ using both the 4 and 8 Torr data sets. The only available MW data on this molecule are the seven $K = 0$, $J = 0-6$ lines from Lide. We therefore had to use the present data to determine a new set of ground state constants that included centrifugal distortion terms for this molecule. We compare these experimentally determined values with both Lide’s A, B, C values and the recent calculated ab initio values of Villa, Senent & Carvajal. Upper state constants have also been been derived that provide a good simulation of the observed spectra. The hope is that this data will be useful in identifying isotopic propane lines in Titan and other astrophysical objects.

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