

FIRST HIGH RESOLUTION IR SPECTRA OF 2-D₁-PROPANE. THE ν_9 (A₁) 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 ¹³C 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 ν_{26} (B₂) C-Type band whose corresponding band in C₃H₈ 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 ν_9 (A₁) 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.^a 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.^b 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.^c Upper state constants have also 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.

^aC. Western, *J. Quant. Spectrosc. & Rad. Transf.* **186**, 221 ff. (2017).

^bLide, *J. Chem. Phys.* **33**, p.1514ff. (1960).

^cVilla, Senent & Carvajal, *PCCP* **15**, 10258 (2013).