High resolution analysis of the ν_{26} and $2\nu_9 - \nu_9$ bands of propane: Modeling of Titan's infrared spectrum at $13.4 \mu\text{m}$

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High resolution analysis of the ν_{26} and $2\nu_9 - \nu_9$ bands of propane: Modeling of Titan's infrared spectrum at 13.4 μm

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Abstract

Using high-resolution Fourier transform spectra of propane recorded in the 13.4 μm (resolution of 0.002 cm^{-1}) and in the 27.4 μm (resolution 0.0011 cm^{-1}) spectral regions, it was possible to perform a thorough assignment of both the ν_{26} band at 745 cm^{-1} and the $2\nu_9 - \nu_9$ band at about 370 cm^{-1} . This simultaneous assignment was necessary since the 26^1 and 9^2 rotational levels interact strongly through an A-type Coriolis interaction. The experimental upper-state rotational levels were fit using a Hamiltonian matrix which takes into account explicitly this strong A-type Coriolis interaction. With this model the experimental energy levels were fit to within their experimental uncertainties and accurate band centers, rotational, centrifugal distortion and coupling constants were determined. The following band centers were derived: $\nu_0(\nu_{26}) = 748.530882(80) \text{ cm}^{-1}$ and $\nu_0(2\nu_9) = 740.29213(10) \text{ cm}^{-1}$. Finally, we show how the use of these new spectral parameters greatly improves the accuracy of modeling of Titan's infrared spectrum at 13.4 μm , relative to the currently available GEISA atlas for the same band.

I. Introduction

The 13.4 μm absorption region of propane is of very high interest since this is the spectral region that led to the first detection of this molecule in the atmosphere of the giant planets [1,2] and Titan [3]. Note as well that the 748 cm^{-1} band has been exclusively and extensively used to derive the abundance and/or concentration profiles of propane in the Titan atmosphere (see for example refs. [4-6]). In fact, it is only recently that other spectral regions have been used for this purpose [7]. The propane absorption at $13.4\text{ }\mu\text{m}$ is mostly due to the ν_{26} band [8]. It has been studied at high resolution using a tunable diode laser spectrometer and analyzed assuming that the 26^1 vibrational state was isolated [9]. In this case such an assumption was valid given the J and K_a range of the observed transitions.

In this paper, we present an extensive analysis of the $13.4\text{ }\mu\text{m}$ absorption region of propane combined with an analysis of the $27.4\text{ }\mu\text{m}$ region. It was necessary to work simultaneously in these two spectral regions since the 26^1 ro-vibrational levels interact strongly with the 9^2 ro-vibrational level through an intense A-type Coriolis resonance. While the 26^1 rotational levels were observed in the $13.4\text{ }\mu\text{m}$ spectral domain, the 9^2 rotational levels were derived from assigning the $2\nu_9 - \nu_9$ hot band in the $27.4\text{ }\mu\text{m}$ spectral region. The $2\nu_9$ band is quite weak and cannot be observed at $13.4\text{ }\mu\text{m}$ except where the 9^2 levels resonate with 26^1 levels.

Propane is an asymmetric top with C_{2v} symmetry. Its structure and symmetry properties are given in Fig. 1 of ref. [10].

II. Experimental details

The high-resolution absorption spectrum of propane was recorded using the Bruker IFS 125HR Fourier transform spectrometer¹ (an upgraded version of the IFS 120HR) at LISA in Créteil. The spectrometer was equipped with a Globar source, a Ge/KBr beamsplitter and a MCT photovoltaic detector cooled by liquid nitrogen. The Fourier transform spectrometer (FTS) was

¹ Certain commercial equipment instruments or materials are identified in this paper to adequately specify the experimental procedure. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

evacuated down to 6.7 Pa (0.05 Torr) pressure (to minimize residual H₂O and CO₂ absorption in the spectra), and a 1.3 mm entrance aperture diameter was used. The spectrum was the result of the co-addition of 600 interferograms collected with a Maximum Optical Path Difference (MOPD) of 450 cm (which corresponds to a resolution of 0.002 cm⁻¹, as defined by Bruker) and was not numerically apodized.

The White-type multipass absorption cell, made of pyrex glass and equipped with CsBr windows, was connected to the FTS with a dedicated optical interface (six mirrors) inside the sample chamber of the FTS. Its base length is 0.80 m, and, for the experiment described here, an optical path of 19.2 m was used. The sample of propane was obtained from Sigma Aldrich. The chemical purity of propane was specified to 99.97% and was used without further purification. The absorption cell was evacuated and filled with 273.6 (7) Pa (2.052 (5) Torr) of pure propane. Sample pressure in the cell was measured using calibrated MKS Baratron gauge (accuracy of 0.25%) with a full scale reading of 10 Torr. The White-type long path cell was at a room temperature of 22 °C.

The spectrum was calibrated with residual CO₂ and H₂O lines observed in the spectrum between 600 and 1400 cm⁻¹, with their wavenumbers taken respectively from HITRAN04 [11] and Toth [12]. The spectral calibration is accurate to within 0.0003 cm⁻¹ (RMS).

Fig. 1 gives an overview of the propane spectrum showing the high signal-to-noise ratio which was obtained. The distinctive shape of the C-type ν_{26} band with its narrow Q-branch is easily recognizable.

III. Analysis and results

The assignment process was started using the upper state constants of [9] and considering 26¹ as an isolated vibrational state. It was possible to assign transitions with low and medium J and K_a quantum numbers rather easily. However, as soon as K_a values around 15 and 16 were reached, it appeared that the predicted positions obtained using a single Watson-type Hamiltonian were incorrect; the predictions clearly became worse with increasing K_a values. Looking for possible interacting states, one option was to consider an A-type Coriolis interaction between the rotational levels of the 26¹ and 9² vibrational states. The corresponding Hamiltonian matrix is given in Table 1. As preliminary band centers and rotational and centrifugal distortion constants for the 9² state, we extrapolated the values previously obtained for the 9¹ state [13]. In this way, high K_a transitions of ν_{26} could better predicted and confidently assigned. As a result, good predictions could be made for the

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2 $2\nu_9$ transitions with K_a values ranging from 18 to 23. These transitions could be observed and
3 together with the ν_{26} transitions were fitted using the two state model (Table 1). Note that these $2\nu_9$
4 transitions could be observed only because they borrow their intensity from the strong resonating ν_{26}
5 lines. In fact, $2\nu_9$ is very weak and no other transitions belonging to this band could be observed at
6 $13.4\ \mu\text{m}$. We then decided to look for the $2\nu_9 - \nu_9$ hot band located at about $370\ \text{cm}^{-1}$. At room
7 temperature this band has an intensity of about 33% of the corresponding cold band, ν_9 . Assigning
8 this hot band proved to be not too difficult given the previous assignments at $13.4\ \mu\text{m}$ and the quality
9 of the model. We worked simultaneously in both regions until it was not possible to assign any
10 additional new lines.
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15 Table 2 gives the number of levels and the range of quantum numbers, J and K_a which were
16 observed for both states. These levels were fit using the two state Hamiltonian model given in Table
17 1. The fit is quite nice as can be seen from the statistical analysis of Table 2 and the standard
18 deviation of $0.41 \times 10^{-3}\ \text{cm}^{-1}$. The corresponding spectroscopic constants are given in Table 3. Using
19 these spectroscopic constants, we have generated a line list of positions and intensities for the ν_{26}
20 and $2\nu_9$ bands at $13.4\ \mu\text{m}$ and for the $2\nu_9 - \nu_9$ hot band at $27.4\ \mu\text{m}$. Fig. 1 presents a simulation of the
21 entire $13.4\ \mu\text{m}$ region showing the good agreement between the observed and calculated spectra.
22 Note the appearance of hot bands around 749.5 and $750.9\ \text{cm}^{-1}$ which are not included in the
23 simulation. Fig. 2 shows a portion of the ν_{26} spectrum where high K_a R transitions are clearly visible.
24 One high K_a R transition of $2\nu_9$ is seen in the spectrum. We note that these $2\nu_9$ transitions can be
25 seen only because high K_a levels of 9^2 resonate with high K_a levels of 26^1 through a strong A-type
26 Coriolis resonance. Finally, in Fig. 3 the PQ_9 -branch of the hot band $2\nu_9 - \nu_9$ is clearly visible. In all
27 cases the agreement between simulation and observation is quite good showing the quality of the
28 simulations.
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36 **IV. Application to Titan**

37 Recently, Titan's mid-infrared spectrum was searched for the presence of multiple propane
38 bands [7], using data recorded by the Cassini Composite Infrared Spectrometer [15]. This research
39 demonstrated that at least five further bands are now clearly detected, in addition to the ν_{26} band
40 traditionally used to measure propane in outer planet atmospheres, and providing the opportunity to
41 make multiple independent estimates of the abundance of the gas. Using a newly-available line list
42 for several bands near $7\ \mu\text{m}$ [10], Nixon et al. made the first measurement of propane's abundance
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via the ν_{18} band at $7.3 \mu\text{m}$, applied to Titan low-latitude limb data, comparing it to a simultaneous measurement using the ν_{26} band. The resulting abundances (Volume mixing ratio (VMR)): $(5.7 \pm 0.8) \times 10^{-7}$ and $(4.2 \pm 0.5) \times 10^{-7}$ respectively did not quite overlap at $1-\sigma$ level of error, and in addition it was clear that the GEISA 2003 spectral data [16] used to model the ν_{26} was not fitting all the propane emission, especially a suspected hot band on the short wavelength side of the main band.

We have therefore sought to check whether the new parameters for the ν_{26} and other bands at $13.4 \mu\text{m}$ improve the fitting of the Titan spectrum in this region, using the same dataset and model as [7]. Fig. 4 shows the comparison between the Titan spectrum (0.5 cm^{-1} apodized resolution) and three models (see [7] for details), including a no-propane model for reference. It is immediately apparent that the new propane list² provides a significantly improved fit to the spectrum (χ^2/n reduces from 6.9 to 2.4) especially in the hot band emission centered near 749.75 cm^{-1} . Moreover, the inferred abundance in VMR of propane at 2 mbar increases by a factor of ~ 1.6 to $(6.6 \pm 0.7) \times 10^{-7}$, reducing the discrepancy with the ν_{18} band from -1.5×10^{-7} , to $+0.9 \times 10^{-7}$ – an agreement finally to within the predicted measurement error.

V. Conclusion

A complete and simultaneous analysis of high-resolution Fourier transform spectra recorded in the 748 and 370 cm^{-1} regions has permitted the assignment of a large number of transitions of the ν_{26} and $2\nu_9$ bands of propane at $13 \mu\text{m}$ and of the accompanying hot band $2\nu_9 - \nu_9$ at $27.4 \mu\text{m}$. A set of accurate spectroscopic constants was obtained for both upper states using a two state Hamiltonian model taking explicitly into account the strong A-type Coriolis interaction linking the rotational levels of the 26^1 and 9^2 vibrational states. Application of the new line list to the modeling of a low-latitude Titan spectrum significantly improves the fitting between model and data relative to the publicly available GEISA data, and should provide a substantial increase in accuracy for researchers using the ν_{26} band to measure propane's abundance in planetary atmospheres.

Acknowledgments

² The linelist can be obtained from the authors..

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Captions to figures

Fig. 1. Overview of the ν_{26} band of propane. The distinctive shape of this typical C-type band is clearly visible.

Fig. 2. High K_a lines of the ν_{26} band of propane. The $2\nu_9$ line is visible only because it borrows its intensity from ν_{26} through a strong A-type Coriolis resonance.

Fig. 3. The PQ_9 -branch of the $2\nu_9 - \nu_9$ hot band of propane. The lines marked with a * belong to the ν_9 cold band [11]. All the $2\nu_9 - \nu_9$ lines are well modeled.

Fig. 4. Upper panel: Titan spectral average, 30°S-30°N latitude, 100-150 km detector centers (black line) compared to three models: (i) no propane, C_2H_2 , C_2H_6 and HCN only (blue); (ii) GEISA 2003 propane atlas (green); (iii) propane atlas from this work (red). Lower panel: the data-model residual. Note that the GEISA 2003 atlas lacks the hot band emission at 749.75 cm^{-1} that is fitted in the new model.

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List of Tables

Table 1: Hamiltonian matrix used to calculate the $\{26^1, 9^2\}$ interacting states of propane.

Table 2: Range of quantum numbers observed for experimental energy levels of the vibrational states 26^1 and 9^2 of propane.

Table 3: Vibrational band centers, rotational and Coriolis interaction constants (in cm^{-1}) for the $\{26^1, 9^2\}$ interacting states of propane.

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Table 1

	26^1	9^2
26^1	H_W	Herm conj
9^2	C^A	H_W

v-diagonal operators:

$$H_W = E_v + [A^v - \frac{1}{2}(B^v + C^v)]J_z^2 + \frac{1}{2}(B^v + C^v)J^2 + \frac{1}{2}(B^v - C^v)J_{xy}^2$$

$$-\Delta_K^v J_z^4 - \Delta_{JK}^v J_z^2 J^2 - \Delta_J^v (J^2)^2 - \delta_K^v \{J_z^2, J_{xy}^2\} - 2\delta_J^v J_{xy}^2 J^2$$

$$+ H_K^v J_z^6 + H_{KJ}^v J_z^4 J^2 + H_{JK}^v J_z^2 (J^2)^2 + H_J^v (J^2)^3$$

$$+ h_K^v \{J_z^4, J_{xy}^2\} + h_{KJ}^v \{J_z^2, J_{xy}^2\} J^2 + 2h_J^v J_{xy}^2 (J^2)^2$$

$$+ L_K^v J_z^8 + L_{KKJ}^v J_z^6 J^2 + L_{KJ}^v J_z^4 (J^2)^2 + L_{JK}^v J_z^2 (J^2)^3 + L_J^v (J^2)^4$$

$$+ l_K^v \{J_z^6, J_{xy}^2\} + l_{KJ}^v \{J_z^4, J_{xy}^2\} J^2 + l_{JK}^v \{J_z^2, J_{xy}^2\} (J^2)^2 + 2l_J^v J_{xy}^2 (J^2)^3$$

$$+ P_K^v J_z^{10} + P_{KKKJ}^v J_z^8 J^2 + P_{KKJ}^v J_z^6 J^4 + \dots$$

v-off-diagonal operators:

$$C^A = h_1^A J_z + h_2^A \{i J_y, J_x\} + h_3^A J_z J^2 + h_4^A \{\{i J_y, J_x\}, J_z^2\}$$

$$\text{with } \{A, B\} = AB + BA, J_{\pm} = J_x \mp i J_y \text{ and } J_{xy}^2 = J_x^2 - J_y^2$$

Table 2

Vibrational State	26 ¹	9 ²
Number of levels	1062	741
J _{max}	58	46
K _{max}	31	26
0.0000≤δ<0.0003	78.5%	70.6%
0.0003≤δ<0.0006	13.3%	18.1%
0.0006≤δ<0.0012	6.4%	7.3%
0.0004≤δ<0.0035	1.8%	4.0%
Std, Deviation (10 ⁻³ cm ⁻¹)	0.41	

$\delta = |E_{\text{Obs.}} - E_{\text{Calc}}| \text{ in cm}^{-1}$

Table 3

	0^0	26^1	g^2
E_v		748.530882(80)	740.29213(10)
A	0.9742562313 ^a	0.97455697 (170)	0.99582808(210)
B	0.2817271865	0.280898922(500)	0.281336087(650)
C	0.2488055608	0.248098043(410)	0.247503322(560)
$\Delta_K \times 10^6$	5.324721011	5.356984 (5000)	6.799600(8900)
$\Delta_{JK} \times 10^7$	-8.998168326	-8.85088(2500)	-8.49929(2100)
$\Delta_J \times 10^7$	2.402258565	2.389984(2300)	2.346993(3200)
$\delta_K \times 10^7$	1.035202827	1.1900(1500)	6.6482(3000)
$\delta_J \times 10^8$	4.659136555	4.69748(1300)	4.67524(2000)
$H_K \times 10^{10}$	1.147493844	1.20062(4600)	2.20292(9100)
$H_{KJ} \times 10^{11}$	-4.071816910	-4.6480(3700)	b
$H_{JK} \times 10^{13}$	5.193592962	b	b
$H_J \times 10^{13}$	2.755239426	b	b
$h_K \times 10^{12}$	-2.568443533	b	b
$h_{KJ} \times 10^{12}$	1.377953277	b	b
$h_J \times 10^{13}$	1.197995448	b	b
$L_K \times 10^{15}$	-2.625149429	b	b
$L_{KKJ} \times 10^{16}$	4.703253742	b	b
$L_J \times 10^{19}$	-7.104915228	b	b

$\langle g^2 26^1 \rangle$	
h_1^A	$0.4458926(1400) \times 10^{-1}$
h_2^A	$0.4739(1700) \times 10^{-5}$
h_3^A	$0.98996(2000) \times 10^{-6}$
h_4^A	$-0.20140(9000) \times 10^{-6}$

^a Ground state values from ref. [14].^b Fixed at ground state values.^c Uncertainties are 1σ .

Overview of the ν_{26} band of propane

Absorbance

Wavenumber (cm^{-1})

High K_a lines of the ν_{26} band of propane

The pQ_9 -branch of the $2\nu_9-\nu_9$ hot band of propane

1322x1763mm (72 x 72 DPI)