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Relative high-resolution absorption cross sections of C_2H_6 at low temperatures

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ABSTRACT

Synchrotron radiation has been used to record absorption cross sections of ethane, C_2H_6, in the far-infrared with very high spectral resolution (up to 0.00096 cm^{-1}). C_2H_6 is present in the atmospheres of the Gas Giant planets and Titan but the vapor pressure at relevant atmospheric temperatures (i.e., between 70 and 200 K) is low. This makes laboratory measurements difficult. We demonstrate the effectiveness of a unique "enclosive flow" cold cell, located at the Australian Synchrotron, that enables high-resolution absorption cross sections of gaseous C_2H_6 to be recorded at 90 K.

1. Introduction

Remote sensing can be used to determine the physical and chemical properties of the outer planets and their satellites. Current instruments, such as the Composite Infrared Spectrometer (CIRS) aboard the Cassini space probe [1], make use of spectroscopic databases for retrievals. This is done by matching an observed planetary spectrum to a calculated spectrum from a forward radiative transfer model with assumed parameters as a function of altitude (e.g., temperature, pressure and composition). Thus, remote sensing is entirely dependent on the availability of suitable spectroscopic data.

The spectroscopic data are generally available as either line parameters or absorption cross sections. Line parameters for small molecular species (e.g., H_2O) can be found in spectroscopic databases, such as HITRAN [2], which have been compiled for the study of the Earth's atmosphere. However, line parameters are not available for all molecules over the complete spectral range of remote sensing instruments (e.g., CIRS covers 10–1400 cm^{-1}), and for larger molecular species (e.g., benzene) it is typically more appropriate to use absorption cross sections due to the blended nature of the infrared spectrum.

Ethane (C_2H_6) is responsible for prominent features in the spectra of the outer planets, comets and Titan. C_2H_6 has 12 vibrational modes, of which only 5 are infrared active (D_{3d} symmetry). Complete line assignments are difficult to obtain partly due to the low-lying torsional mode (ν_4) near 35 μm (290 cm^{-1}) [3–6]. This leads to a large number of low frequency hot bands, extensive perturbations and a very dense line structure. To date, the ν_9 mode near 12 μm (830 cm^{-1}) contains the most complete assignments due to extensive work reported in references [7–9]. Recent line parameters and partial assignments have also been provided for the ν_8 band near 6.8 μm (1470 cm^{-1}) [10,11] as well as the 3.3 μm (3000 cm^{-1}) region that contains the ν_5 and ν_7 modes [12,13]. Although considerable progress has been made in these recent studies, high-resolution analyses generally still fail to match laboratory observations precisely.

The Pacific Northwest National Laboratory (PNNL) has recorded infrared absorption cross sections for a large number of species, including C_2H_6 (see http://nwir.pnl.gov and [14]). These spectra cover the 600–6500 cm^{-1} spectral range; however, these data are not always suitable for remote sensing of planetary atmospheres because of the temperature (278, 293 and 323 K), pressure (760 Torr of N_2) and resolution (0.112 cm^{-1}) at which the data were recorded. The main problem with using relatively low resolution absorption cross sections is that spectroscopic features (e.g., sharp Q-branches) are under-resolved and give incorrect radiative transfer. Due to these issues, Harrison et al. [15] have provided high-resolution infrared cross sections of the 3.3 μm band intended for retrievals of terrestrial C_2H_6 from atmospheric observations. Whilst these measurements extend the absorption

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cross sections of C_2H_6 to lower temperatures, the air-broadened spectra are unsuitable for planetary retrievals. Nixon et al. [16] highlighted the importance of reliable high-resolution spectroscopic data for planetary retrievals by observing propene (C_3H_6) in the atmosphere of Titan. This was made possible after the removal of propane (C_3H_8) by using the latest absorption cross sections obtained from a series of N_2-broadened spectra at temperatures as low as 145 K [17].

The primary constituents of the atmospheres of Jupiter and Saturn are hydrogen and helium, approximately 86% H_2 and 14% He for Jupiter and 88% H_2 and 12% He for Saturn (by mole fraction [18]). In each case, trace gases account for less than 1% of the atmosphere, of which methane is the most abundant ($\sim 0.3\%$), but C_2H_6 provides a detectable contribution ($\sim 0.0004\%$). The atmospheric profiles of Jupiter and Saturn demonstrate that the majority of C_2H_6 is found at a typical temperature range of around 70–200 K [19].

Titan is the only moon in the Solar System with an appreciable atmosphere, approximately 95% N_2 and 5% CH_4 at a total pressure of 1.5 atm at the surface [20,21]. The trace species are mainly hydrocarbons formed from the photolysis of CH_4 [22] and subsequent reactions, as is the case for C_2H_6 [23]. In Titan, the atmospheric profile indicates that the majority of C_2H_6 is found at a typical temperature of 70–180 K [19], and pressures between 0.075 and 75 Torr ($\sim$ 40–300 km) [24].

Hence, it would be appropriate to have cross-sections of C_2H_6 over a temperature range 70–200 K that are broadened by H_2 and He (Jupiter and Saturn) as well as N_2 (Titan). Absorption cross sections of C_2H_6 have not previously been provided over the complete temperature range due to the low vapor pressure at low temperatures (< 1 Torr below 110 K [25]). Planetary atmospheres provide extremely long effective path lengths that are difficult to obtain and often impractical for laboratory conditions. Conventional cooling of the gas typically leads to the C_2H_6 condensing on the cell walls.

The aim of this work is to provide high-resolution cross sections of C_2H_6 that includes all of the fundamental bands over the appropriate temperature ranges and conditions of the outer planets and Titan. This will be completed using a Fourier transform spectrometer (FTS), cold cell and infrared source at Old Dominion University (ODU) as well as with synchrotron sources. This paper introduces our latest experiments at the Australian Synchrotron (AS), which provides the necessary source and cell to enable high-resolution absorption cross sections to be recorded at temperatures and ranges that are difficult or excessively time consuming to obtain using the equipment available at ODU.

2. Synchrotron radiation

Synchrotron radiation has a number of advantages over a traditional radiation source (typically a glower) when recording high-resolution spectra in the far/mid infrared region using an FTS [26]. Many benefits will be discussed in this special issue, but only key improvements are mentioned here.

The narrow intense beam provided by a synchrotron allows small apertures to be used, and therefore high spectral resolutions. The signal-to-noise at wavelengths longer than 10 μm is improved by at least a factor of three when compared to a glower. Since the signal-to-noise ratio increases as the square root of integration time, this leads to a reduction in acquisition time by almost a factor of 10. Due to the large number of spectra that are required to obtain high-resolution infrared cross sections at relevant temperatures and pressures, synchrotron radiation is a valuable (and under-exploited) source for absorption cross sections of vibrational bands at wavelengths longer than 10 μm.

3. Measurements

The Far IR/THz beamline of the AS provides a Bruker IFS 125 spectrometer with a maximum optical path difference (MOPD, Δ) of 9.3 m and therefore, a maximum resolution $R = 0.00096\ \mathrm{cm}^{-1}$ is possible ($R \sim 0.9/\Delta$ using the Bruker definition). The AS also has unique access to a cooled gas cell that has been designed to record spectra of gases at low temperatures [27] based on a cell designed for supercooling molecular clusters [28]. The cell can be used in two operating modes depending on the temperature and gas of interest. The standard static mode is when the sample gas is sealed within the cell at fixed pressure during measurements. The second mode is known as "Enclosive Flow Cooling" (EFC) and is achieved by enclosing the sample gas within a laminar flow of buffer gas to avoid condensation on the cell walls. The enclosive conditions are created by introducing the sample gas at the center of a vertical cell with an exhaust at the base. A buffer gas is introduced to the cell from all directions as it has to pass through a cylinder with holes (the colander) before reaching the exhaust. The gases are drawn through the cell by the exhaust, thus creating a columnar laminar flow that constrains the sample gas to the center of the cylinder (see reference [27] for diagram). The EFC cell has a maximum path length of 20 m, but since the sample gas is rapidly cooled by the buffer gas without freezing out on the walls, the enclosive mode allows spectra to be acquired that are more typical of longer path lengths (e.g., planetary atmospheres) at low temperatures.

The AS is crucial for measurements at wavenumbers below $1000\ \mathrm{cm}^{-1}$ particularly at low temperatures (< 110 K) since the natural vapor pressure of C_2H_6 requires long path lengths (e.g., enclosive flow measurements). Temperatures as low as 200 K can be reached at ODU using a static ethanol cooled cell with a 20 cm path length [29]. The MOPD for the Bruker spectrometer at ODU is 4.3 m, corresponding to a spectral resolution of $0.0021\ \mathrm{cm}^{-1}$. For wavenumbers greater than $1000\ \mathrm{cm}^{-1}$, measurements at ODU will be able to reach the sensitivity of synchrotron spectra. However, measurements at wavenumbers less than $1000\ \mathrm{cm}^{-1}$ should be conducted at a synchrotron. Current work is being done at the Canadian Light Source (CLS) to provide a static liquid-N_2 cooled cell that is capable of taking measurements when the C_2H_6 vapor pressure remains relatively high (i.e., $T > 110$ K).

Each PNNL cross section is a composite of approximately ten pathlength concentrations, making these data suitable for calibration. Since the integrated band intensities are independent of temperature, the PNNL data will be used to calibrate our high-resolution cross sections, as done previously [15]. Combining the

Table 1
Summary of the N_2-broadened spectra of C_2H_6 recorded at the Australian Synchrotron with the EFC cell.[a]

Temp (K)	Source	C_2H_6 pressure (Torr)	N_2 pressure (Torr)	Resolution (cm^{-1})	Scans
200	Synchrotron	0.3	0.0	0.003	176
200	Synchrotron	0.5	5.0	0.003	175
200	MIR	1.0	25.0	0.01	400
200	MIR	1.0	100.0	0.04	400
160	Synchrotron	0.2	0.0	0.002	118
160	Synchrotron	0.5	2.0	0.002	119
160	MIR	0.8	25.0	0.01	442
160	MIR	1.0	100.0	0.04	400
120	Synchrotron	0.1	0.0	0.00096	294
120	Synchrotron	0.1	5.0	0.002	322
120	MIR	0.5	25.0	0.01	500
120	MIR	0.6	100.0	0.04	400
90	Synchrotron	< 0.05	5.0	0.002	80
90[b]	Synchrotron	< 0.05	5.0	0.002	80

[a] Path length of 2 m.
[b] Enclosive conditions.

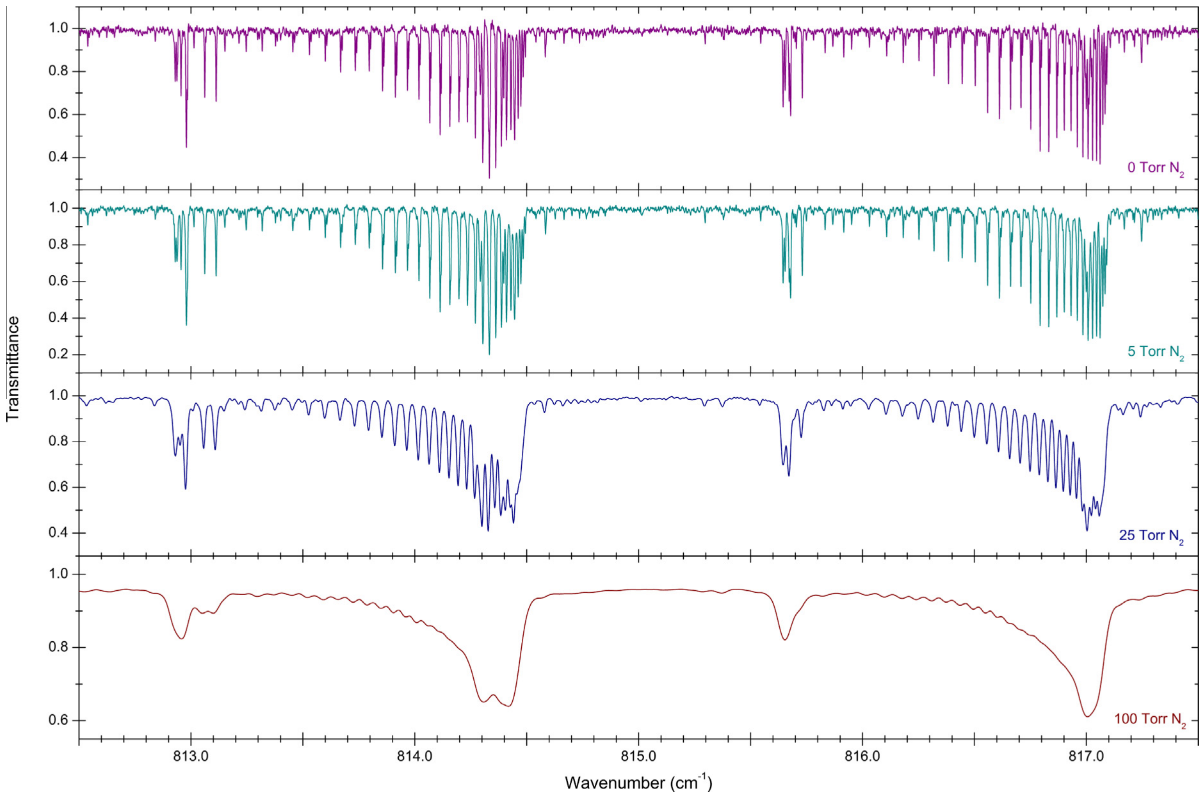

Fig. 1. The $^PQ_3$ and $^PQ_2$ sub-bands of C_2H_6 at 200 K. The spectra were recorded at the Australian Synchrotron using the Enclosive Flow Cooling cell in static mode with 1 Torr of C_2H_6 and varying pressures of N_2 (as indicated).

spectra from all three locations (ODU, AS and CLS) will enable the high-resolution infrared cross section of C_2H_6 to be provided for all the fundamental bands at the appropriate temperature ranges of the outer planets and Titan.

4. Proof of concept

Measurements were taken at the AS during February 2014 to test the feasibility of the low vapor pressure measurements of C_2H_6. N_2-broadened spectra were taken at four temperatures (200, 160, 120 and 90 K) using the synchrotron and EFC cell. The results cover the appropriate temperature range and atmospheric conditions of Titan and are summarized in Table 1.

Fig. 1 displays the N_2-broadened spectra of C_2H_6 at 200 K and demonstrates the reduction of spectral resolution on the $^PQ_3$ (near 814.5 cm^{-1}) and $^PQ_2$ (near 817.1 cm^{-1}) sub-bands with increasing pressure. The spectra are recorded at a higher resolution than the observed pressure-broadened linewidth (primarily due to N_2-broadening) and a corresponding background spectrum (i.e., empty cell) was recorded to create the transmittance spectra. Reflections in the beamline due to windows and mirrors, required to direct the beam through the EFC cell, result in a strong channeling that causes a sine-like wave to be present in the baseline due to interference. This channeling effect is partly removed by dividing by the background, but a residual effect can be seen in the fluctuating intensities of the highest resolution spectra (top two spectra of Fig. 1).

The cell is cooled and maintained at a specified temperature using the boil-off from liquid-N_2. Measurements at 200, 160 and 120 K demonstrated the feasibility of using the EFC cell in static mode at the temperatures appropriate for the outer planets and Titan. The same cooling method is used to reach a temperature of 90 K where the vapor pressure of C_2H_6 is approximately 0.02 Torr [25]. Fig. 2 displays the spectra of two measurements at 90 K for the $^PQ_1$ sub-band near 819.7 cm^{-1} (described in Table 1). These two spectra demonstrate the significant improvement between enclosive and static modes when using the EFC cell.

5. Discussion

The temperature range observed in the atmospheres of the outer planets and Titan (70–200 K) can prove difficult for some important gases (e.g., C_2H_6 and C_3H_8). When using the EFC cell at the AS in static mode, the vapor pressure of C_2H_6 at 90 K is too low to record a suitable spectrum with a 2 m path length. This paper demonstrates that when using the enclosive technique provided by the EFC cell, spectra can be recorded of C_2H_6 at 90 K.

From spectra of this type, we are able to produce a set of absorption cross sections. It has previously been demonstrated that integrating an absorption cross section over an isolated band comprising primarily of fundamentals exhibits an insignificant temperature dependence [15,30–36]. For the PNNL spectra of C_2H_6 at 278, 293 and 323 K, the integrated absorption cross section between 700 and 960 cm^{-1} is calculated as

$$\int_{700\text{cm}^{-1}}^{960\text{cm}^{-1}} \sigma(\nu,T)d\nu = 1.014(\pm 0.003) \times 10^{-18}\ \text{cm molecule}^{-1}, \quad (1)$$

with less than 0.3% change between temperatures.[1]

Absorption cross sections can be calculated from a transmittance spectrum $\tau(\nu,T)$ as

$$\sigma(\nu,T) = -\xi \frac{10^4 k_B T}{Pl} \ln \tau(\nu,T), \quad (2)$$

[1] PNNL units ($ppm^{-1}\,m^{-1}$ at 296 K) have been converted using the factor $k_B \times 296 \times \ln(10) \times 10^4/0.101325 = 9.28697 \times 10^{-16}$ [35].

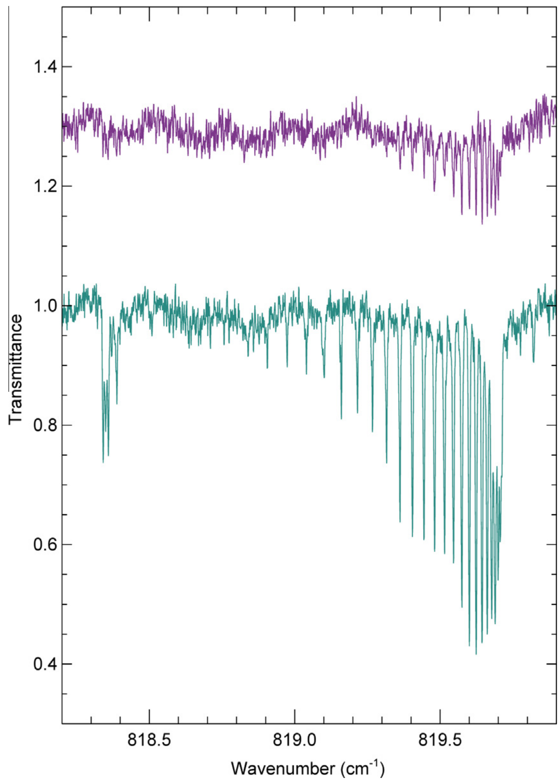

Fig. 2. The $^PQ_1$ sub-band of C_2H_6 at 90 K during non-enclosive (top) and enclosive (bottom) conditions. Spectral parameters are given in Table 1 and the non-enclosive spectrum is offset by 30%.

where v in the wavenumber (cm^{-1}), T is the temperature, k_B is the Boltzmann constant, P is the pressure of the absorbing gas (Pa), l is the optical pathlength (m) and ξ is a normalization factor [15,35]. This procedure is based on the assumption that the integrated band intensity does not vary as a function of temperature and ξ is used to account for the difficulty in determining the amount of absorbing gas with great accuracy. For the static mode observations, the pressure and temperature of the absorbing gas can be recorded and the absorption cross sections can be calculated easily using Eq. 2. However, determining the sample gas pressure for the enclosive measurements is not a simple problem, as the gas is no longer in thermal equilibrium. Therefore, only an effective pressure (P_{eff}) of the column can be determined. Since it is assumed that the integrated band intensity is unchanged, it is possible to calculate P_{eff} for the enclosive measurement at 90 K by assuming $\xi = 1$ and the temperature in the cell is uniform. The EFC cell has been designed to minimize temperature gradients during enclosive flow, but nevertheless a small gradient will remain over the whole pathlength. Whilst this will not greatly affect the integrated absorption intensities, it is worth noting that the measured temperature will actually be an effective temperature and will also need to be considered in the error budget. Analysis of the preliminary 90 K data suggest P_{eff} is greater than measured during the experiment (Table 1) thereby demonstrating the benefit of the enclosive method at temperatures when the vapor pressure is low, such as C_2H_6 at 90 K. These measurements are preliminary and further measurements are necessary to produce acceptable cross sections.

These absorption cross sections could be used directly at the temperature the spectra were recorded (i.e., 200, 160, 120 and 90 K) or the cross sections can be regenerated from a set of line parameters. The line parameters can be obtained through extensive analysis, for example by using a multispectrum nonlinear least squares analysis technique [37], as used previously for C_2H_6 [8,9]. Another way to obtain line parameters is by using a set of pseudolines, which are provided on a frequency grid and are treated as if they are real transitions [38,39]. These pseudolines are then able to reproduce the cross sections over the temperature range as demonstrated for C_3H_8 [17].

The measurements presented here will be expanded to provide cross sections of the fundamental bands of C_2H_6 for remote sensing of the outer planets and Titan. These cross sections will cover the appropriate atmospheric temperatures (70–200 K) and will include the relevant broadening gases (H_2 and He for the Gas Giants, N_2 for Titan). We intend to continue the EFC measurements for molecules that have low vapor pressures at warmer temperatures than for C_2H_6. One example is C_3H_8, which has a vapor pressure of < 1 Torr at 140 K [25].

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References

[1] F.M. Flasar, V.G. Kunde, M.M. Abbas, R.K. Achterberg, P. Ade, A. Barucci, et al., Space Sci. Rev. 115 (2004) 169–297, http://dx.doi.org/10.1007/s11214-004-1454-9.
[2] L.S. Rothman, I.E. Gordon, Y. Babikov, A. Barbe, D. Chris Benner, P.F. Bernath, et al., J. Quant. Spectrosc. Radiat. Transfer 130 (2013) 4–50, http://dx.doi.org/10.1016/j.jqsrt.2013.07.002.
[3] N. Moazzen-Ahmadi, J. Schroderus, A.R.W. McKellar, J. Chem. Phys. 111 (1999) 9609–9617, http://dx.doi.org/10.1063/1.480294.
[4] N. Moazzen-Ahmadi, E. Kelly, J. Schroderus, V.M. Horneman, The high-resolution far-infrared torsional spectrum of ethane, J. Mol. Spectrosc. 209 (2001) 228–232, http://dx.doi.org/10.1006/jmsp.2001.8427.
[5] L. Borvayeh, N. Moazzen-Ahmadi, V.M. Horneman, J. Mol. Spectrosc. 250 (2008) 51–56, http://dx.doi.org/10.1016/j.jms.2008.04.009.
[6] N. Moazzen-Ahmadi, J. Norooz Oliaee, I. Ozier, E.H. Wishnow, K. Sung, T.J. Crawford, et al., J. Quant. Spectrosc. Radiat. Transfer 151 (2015) 123–132, http://dx.doi.org/10.1016/j.jqsrt.2014.09.016.
[7] J. Vander Auwera, N. Moazzen-Ahmadi, J.M. Flaud, Astrophys. J. 662 (2007) 750–757, http://dx.doi.org/10.1086/515567.
[8] V. Malathy Devi, C.P. Rinsland, D. Chris Benner, R.L. Sams, T.A. Blake, J. Quant. Spectrosc. Radiat. Transfer 111 (2010) 1234–1251, http://dx.doi.org/10.1016/j.jqsrt.2009.10.017.
[9] V. Malathy Devi, D.C. Benner, C.P. Rinsland, M.A.H. Smith, R.L. Sams, T.A. Blake, et al., J. Quant. Spectrosc. Radiat. Transfer 111 (2010) 2481–2504, http://dx.doi.org/10.1016/j.jqsrt.2010.07.010.
[10] F. Lattanzi, C. di Lauro, J.V. Auwera, Mol. Phys. 109 (2011) 2219–2235, http://dx.doi.org/10.1080/00268976.2011.604353.
[11] C. di Lauro, F. Lattanzi, L.R. Brown, K. Sung, J. Vander Auwera, A.W. Mantz, et al., Planet. Space Sci. 60 (2012) 93–101, http://dx.doi.org/10.1016/j.pss.2011.01.008.
[12] G.L. Villanueva, M.J. Mumma, K. Magee-Sauer, J. Geophys. Res. (Planet.) 116 (2011) E08012, http://dx.doi.org/10.1029/2010JE003794.
[13] F. Lattanzi, C. di Lauro, J. Vander Auwera, J. Mol. Spectrosc. 267 (2011) 71–79, http://dx.doi.org/10.1016/j.jms.2011.02.003.
[14] S.W. Sharpe, T.J. Johnson, R.L. Sams, P.M. Chu, G.C. Rhoderick, P.A. Johnson, Appl. Spectrosc. 58 (2004) 1452–1461, http://dx.doi.org/10.1366/0003702042641281.
[15] J.J. Harrison, N.D.C. Allen, P.F. Bernath, J. Quant. Spectrosc. Radiat. Transfer 111 (2010) 357–363, http://dx.doi.org/10.1016/j.jqsrt.2009.09.010.
[16] C.A. Nixon, D.E. Jennings, B. Bézard, S. Vinatier, N.A. Teanby, K. Sung, et al., Astrophys. J. Lett. 776 (2013) L14, http://dx.doi.org/10.1088/2041-8205/776/1/L14. 1309.4489.
[17] K. Sung, G.C. Toon, A.W. Mantz, M.A.H. Smith, Icarus 226 (2013) 1499–1513, http://dx.doi.org/10.1016/j.icarus.2013.07.028.
[18] S.K. Atreya, P.R. Mahaffy, H.B. Niemann, M.H. Wong, T.C. Owen, Planet. Space Sci. 51 (2003) 105–112, http://dx.doi.org/10.1016/S0032-0633(02)00144-7.
[19] I.C.F. Mueller-Wodarg, D.F. Strobel, J.I. Moses, J.H. Waite, J. Crovisier, R.V. Yelle, et al., Space Sci. Rev. 139 (2008) 191–234, http://dx.doi.org/10.1007/s11214-008-9404-6.
[20] H.B. Niemann, S.K. Atreya, S.J. Bauer, G.R. Carignan, J.E. Demick, R.L. Frost, et al., Nature 438 (2005) 779–784, http://dx.doi.org/10.1038/nature04122.

[21] F.M. Flasar, R.K. Achterberg, B.J. Conrath, P.J. Gierasch, V.G. Kunde, C.A. Nixon, et al., Science 308 (2005) 975–978, http://dx.doi.org/10.1126/science.1111150.
[22] V.A. Krasnopolsky, Icarus 201 (2009) 226–256, http://dx.doi.org/10.1016/j.icarus.2008.12.038.
[23] E.H. Wilson, S.K. Atreya, J. Phys. Chem. A 113 (2009) 11221–11226, http://dx.doi.org/10.1021/jp905535a.
[24] P.J. Schinder, F.M. Flasar, E.A. Marouf, R.G. French, C.A. McGhee, A.J. Kliore, et al., Icarus 215 (2011) 460–474, http://dx.doi.org/10.1016/j.icarus.2011.07.030.
[25] C. Yaws, Chemical Properties Handbook: Physical, Thermodynamics, Environmental Transport, Safety & Health Related Properties for Organic & Inorganic Chemicals. Chemical engineering books, McGraw-Hill Education, 1999 (ISBN 9780070734012).
[26] A.R.W. McKellar, J. Mol. Spectrosc. 262 (2010) 1–10, http://dx.doi.org/10.1016/j.jms.2010.04.006.
[27] D.R.T. Appadoo, E.G. Robertson, D. McNaughton, J. Mol. Spectrosc. 217 (2003) 96–104, http://dx.doi.org/10.1016/S0022-2852(02)00030-9.
[28] S. Bauerecker, M. Taraschewski, C. Weitkamp, H.K. Cammenga, Rev. Sci. Instrum. 72 (2001) 3946–3955, http://dx.doi.org/10.1063/1.1400158.
[29] K.A. Tereszchuk, P.F. Bernath, J. Quant. Spectrosc. Radiat. Transfer 112 (2011) 990–993, http://dx.doi.org/10.1016/j.jqsrt.2010.12.003.
[30] B. Crawford Jr., J. Chem. Phys. 29 (1958) 1042–1045, http://dx.doi.org/10.1063/1.1744652.
[31] I.M. Mills, D.H. Whiffen, J. Chem. Phys. 30 (1959) 1619–1620, http://dx.doi.org/10.1063/1.1730254.
[32] J.C. Breeze, C.C. Ferriso, C.B. Ludwig, W. Malkmus, J. Chem. Phys. 42 (1965) 402–406, http://dx.doi.org/10.1063/1.1695707.
[33] S.J. Yao, J. Overend, Spectrochim. Acta Part A: Mol. Spectrosc. 32 (1976) 1059–1065, http://dx.doi.org/10.1016/0584-8539(76)80290-5.
[34] R.L. Sams, S.W. Sharpe, T.J. Johnson, Do integrated infrared band strengths change with temperature in the gas-phase? 2005, in: 60th International Symposium on Molecular Spectroscopy, Columbus, Ohio, US.
[35] J.J. Harrison, N.D.C. Allen, P.F. Bernath, J. Quant. Spectrosc. Radiat. Transfer 113 (2012) 2189–2196, http://dx.doi.org/10.1016/j.jqsrt.2012.07.021.
[36] J.J. Harrison, P.F. Bernath, J. Quant. Spectrosc. Radiat. Transfer 111 (2010) 1282–1288, http://dx.doi.org/10.1016/j.jqsrt.2009.11.027.
[37] D.C. Benner, C.P. Rinsland, V. Malathy Devi, M.A.H. Smith, D. Atkins, J. Quant. Spectrosc. Radiat. Transfer 53 (1995) 705–721, http://dx.doi.org/10.1016/0022-4073(95)00015-D.
[38] K. Strong, F.W. Taylor, S.B. Calcutt, J.J. Remedios, J. Ballard, J. Quant. Spectrosc. Radiat. Transfer 50 (1993) 363–429, http://dx.doi.org/10.1016/0022-4073(93)90072-P.
[39] G.C. Toon, J.F. Blavier, B. Sen, J.J. Margitan, C.R. Webster, R.D. May, et al., J. Geophys. Res.: Atmos. 104 (1999) 26779, http://dx.doi.org/10.1029/1999JD900379.