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A B S T R A C T

The rovibrational spectrum of the v_{14} CH$_3$-bending mode of dimethyl sulfide CH$_3$SCH$_3$ was recorded in the 945–1005 cm^{-1} spectral region combining data from a tunable infrared quantum cascade laser spectrometer coupled to a pulsed slit jet and from a high resolution Fourier transform spectrometer coupled to a room temperature gas absorption cell. The characteristic PQR band contour of a vibrational mode with a b_1 symmetry species in the C_{2v} group was observed with both infrared methods but the rovibrational cooling achieved in the pulsed supersonic expansion (20 K in rotation) proved to be essential for starting the rovibrational analysis of such asymmetric top molecule. Internal rotation splittings were recently observed and analyzed in the ground and first torsional excited states. However, they are expected to be very small and could not be resolved in the v_{14} state using our infrared spectroscopic probes. Therefore a classic reduced effective Hamiltonian of an asymmetric rigid rotor was used. Finally, 1119 transitions from both jet-cooled and room temperature experiments were assigned and included in a global fit with J ≤ 29. A total of 9 rovibrational parameters including pure rotational constants as well as quartic centrifugal distortion constants were determined with high accuracy. These parameters can be used to produce a reliable line-list for an atmospheric detection of DMS.

1. Introduction

Recently the ground state of dimethyl sulfide CH$_3$SCH$_3$ (DMS) received a lot of attention for its potential astrophysical interest. DMS is the sulfur analog of dimethyl ether, a relatively abundant molecule in interstellar medium (ISM) [1–4]. It is thus considered as a potentially detectable species, since the detection of sulfur-containing molecules often follows the detection of the corresponding oxygen-analogs [5]. In 2016 Jabri et al. recorded the microwave region, and analyzed 584 transitions belonging to the ground torsional state $v_{15} = 0$ and 18 hot transitions starting from the first excited torsional state $v_{15} = 1$ with J < 30 and with J < 5 respectively [6]. In the FIR range, where only low resolution spectrum was available, these authors also recorded for the first time the torsional band at high resolution using the synchrotron SOLEIL beamline and 578 transitions belonging to the torsional band $v_t =$

$v_{15} = 1 \leftarrow 0$ with J < 27 were assigned and fitted [6]. In 2017 Ilyushin et al. completed this study by extending the assignments and fitting the first and second torsional states of DMS [7]. These microwave and submillimeter wave spectra of dimethyl sulfide provided a very precise set of spectroscopic parameters describing the ground state.

Apart from experimental studies in the ground state, *ab initio* calculations were performed by Senent et al. using high level of theory CCSD/cc-VTZ [8]. This allows the authors to predict rotational and centrifugal distortion constants as well as the torsional splittings for the lowest torsional states (up to about 400 cm^{-1}). Table III of this reference provides the calculated band center and vibrational assignments.

Dimethyl sulfide is also a species of interest for atmospheric studies as it is the most abundant sulfur compounds of biogenic source emitted in the atmosphere [9]. Produced by marine algae DMS represents a large source of sulfur going into the Earth's atmosphere, and therefore it can help drive the formation of clouds, which block solar radiation from reaching the Earth's surface and reflect it back into space. However very little is known

so far about the quantity of DMS formed, about its potential impact on climate and its possible role to offset greenhouse warming [10,11]. Most of the methods used to detect DMS (for example gas chromatography, mass spectrometry [12] or chemiluminescence [13] are either expensive or require that gaseous DMS to be collected and to react with certain chemical substances before the detection using chemiluminescence. Optical detection will be thus an attractive complementary method to measure DMS in the atmosphere.

Any optical detection of DMS in the atmosphere is however highly dependent on the determination of accurate spectroscopic parameters such as line positions and line intensities in the infrared spectral range used. So far only low resolution vibrational spectra were recorded by Fonteyne [14], Durig & Griffin [15] and Durig et al. [16]. The NIST 69 Databasis [17] and the Pacific Northwest National Laboratory [18] spectral database allow us to visualize the low resolution gas phase spectra for DMS between 500 and 6500 cm^{-1}. It is only this year that using the tunable laser absorption spectroscopy (TLAS) technique with an interband cascade laser at 3.3 μm, Li et al. [19] shows the possibility of measuring DMS with a sensitivity of 20 ppb with time resolution of 1 s, and a measurement precision of 21 ppb, very similar to the chemical methods, and opening the door to a quantitative detection of DMS.

The infrared atmospheric window (8–14 μm) is another convenient spectral range to obtain reliable rovibrational signatures of dimethyl sulfide. The present work targets the first high resolution study of the ν_{14} CH$_3$-bending mode and provides line assignments and fit.

2. Experimental details

Dimethyl sulfide (anhydrous, >99%, Aldrich) was used for all experiments without further purification.

The rovibrational spectrum of ν_{14} CH$_3$-bending mode of dimethyl sulfide (DMS) was first recorded at room temperature using a 75 cm stainless cell coupled to the back parallel exit of a IFS Bruker 120 high resolution Fourier transform spectrometer. The strong spectral congestion due to the broad rotational distribution and the presence of hot bands arising from low frequency modes below 300 cm^{-1} require to use a jet-cooled laser spectrometer recently developed in the MONARIS laboratory. This set-up couples an external-cavity quantum cascade laser (EC-QCL) to a pulsed supersonic jet and has already been described in detail in recent papers [20,21]. Only the main characteristics will be presented hereafter.

As evidenced in previous studies, the combined use of very diluted molecular samples seeded in high backing pressures of carrier gas enabled to obtain an efficient rovibrational cooling. Owing to its relatively high pressure (about 500 mbar at room temperature), DMS was cooled between 233 and 253 K in a stainless steel reservoir thanks to an ethanol-LN$_2$ mixture bath. Argon carrier gas bubbled through the compound to generate low concentrations ranging from 1.5 to 4.5% (in pressure). Jet-cooled DMS was produced in a planar supersonic expansion at backing pressures of Argon (Air liquid) of 2 bar. The light source is a continuous-wave room-temperature mode hop-free EC-QCL with a spectral width of 10 MHz, which covers the 930–990 cm^{-1} range (Daylight Solutions). About 8% of the total light is sent through two laser channels for relative and absolute frequency calibrations. Relative frequencies are monitored by measuring the intensity transmitted through a solid germanium etalon with a free spectral range of 490 MHz, to provide a relative frequency scale. Absolute laser frequencies are obtained by measuring the transmission through a 15 cm length reference cell containing a known reference gas at a pressure of about 5 mbar (ethene in the present work). The remaining

light is sent through a multipass optical cavity mounted in the jet chamber, which is evacuated by a 2000 L s^{-1} oil diffusion pump backed by a combination of a 350 m^3 h^{-1} Roots blower and a 40 m^3 h^{-1} rotary pump. The optical configuration used for the present study is an astigmatic cavity composed of two 1.5″ astigmatic mirrors (R = 99.2%, AMAC-36, Aerodyne Research) aligned according to a 182 pass configuration. Three liquid-nitrogen cooled HgCdTe detectors (Judson J15D12) are used to measure the power transmitted through the multipass cavity, the etalon and the reference gas cell. The molecular jet is produced from a pulsed nozzle (General Valve Series 9) by fitting a 0.9 mm diameter pin hole nozzle with two modified industrial blades, forming a 30 mm length × 50 μm width slit opening, and serving as the molecular expansion source. Rovibrationally cooled molecules were probed by the infrared laser light at average distances between 5 and 10 mm from the nozzle exit which represents a good balance between efficient rovibrational cooling and high molecular density for slit jet expansions. Our rapid scan scheme described in details elsewhere is close to the original designs used for high resolution molecular spectroscopy [22]. Fine tuning of the laser frequency over about 0.8 cm^{-1} at a repetition rate of 100 Hz is obtained by a sine wave generated by a Labview code and delivered to a piezoelectric transducer attached to the diffraction grating that ends the external cavity. The intensities transmitted through the supersonic jet, the etalon and the reference gas cell are digitized and recorded simultaneously as a function of time. A baseline-free transmittance through the multipass cavity is then obtained by taking the ratio of the corresponding signals recorded with and without the jet. The procedure for absolute frequency calibration is achieved in real time by measuring the deviation between experimental and HITRAN12 [23] database C$_2$H$_4$ frequencies after each laser sweep to correct the free spectral range value of the etalon fixed at the beginning of each experiment. The accuracy of the frequency calibration is around 0.0001 cm^{-1}. While the line width of the QCL source is typically 10 MHz, the resolution (full-width-at-half-maximum, FWHM) of isolated rovibrational lines achieved with the jet-cooled QCL spectrum is about 130(20) MHz, limited by both residual Doppler broadening at the temperature of the expansion and a small contribution (dependent on mass of carrier gas) from non orthogonal laser and planar jet crossings in the multi pass optical cavity.

3. Experimental results

The PNNL spectral database [18] provides us a global view of the low resolution dimethyl sulfide spectrum over all the infrared range. Strongest fundamental absorptions are located in two middle infrared regions, 1420–1460 cm^{-1} and 2900–3000 cm^{-1}, respectively. However, both regions present serious drawbacks in the perspective of high resolution measurements: the DMS absorption in the 1420–1460 cm^{-1} region is largely masked by atmospheric water absorption unless the path of the laser beam in fully purged with dry air or nitrogen. About the 2900–3000 cm^{-1} region, six stretching CH$_3$ fundamentals were calculated in a spectral window of about 60 cm^{-1} to which should be added first harmonics of several bending CH$_3$ ones falling in the same region [8]. Such a density of vibrational states, not unusual at these high energies, is far from ideal conditions for extracting reliable molecular parameters from rovibrational analysis. Despite weaker fundamental absorptions, we considered that the infrared atmospheric window (8–14 μm) is the more convenient spectral range to obtain reliable rovibrational signatures of dimethyl sulfide. Accounting for the narrow tunability range (10.1–10.75 μm) of our EC-QCL, we targeted the ν_{14} CH$_3$-bending mode calculated at 986 cm^{-1} with an intensity of 3.4 km/mol [8] and observations were made

at 973 cm^{-1} guided by low resolution room temperature cell experiments [24]. In a first step, a series of survey room temperature cell FTIR spectra were recorded using the combination of a globar source, a KBr beamsplitter and a HgCdTe photovoltaic detector equipped with a band pass filter (centered at 1000 cm^{-1}, 180 cm^{-1} full width at half maximum (FWHM)) at different resolutions and pressures of DMS. Knowing that the Doppler FWHM width of DMS is equal to about 0.0015 cm^{-1} at 975 cm^{-1} the best compromise between signal-to-noise ratio and experimental width is obtained for a cell spectrum recorded at a resolution of 0.003 cm^{-1} (boxcar apodized) and a pressure of 2 mbar. The room temperature DMS spectrum displays several rovibrational bands in the 880–1080 cm^{-1} range (Fig. 1): the most intense one, centered at 1032.7 cm^{-1}, displays the characteristic rovibrational band contour without Q branch of a a_1 symmetry-b type band, assignable to the v_5 HCH-bending mode from comparison with *ab initio* calculations [8] and low resolution IR spectra [15]. The weakest one at 901.9 cm^{-1} is likely to correspond to the v_{20} HCH-bending mode, calculated at 908 cm^{-1} with an intensity of 0.3 km/mol [8]. The v_{14} CH$_3$-bending mode is displayed between both bands, with an intense Q branch characteristic of b_1 symmetry in the C_{2v} group for the fundamental band centered at about 975.1 cm^{-1}. A series of red shifted Q branches of hot bands of the type nv_i + v_{14} ← nv_i up to n = 3 is also observed at 973.3, 971.6 and 969.7 cm^{-1} which display an anharmonicity of −1.8(1) cm^{-1}. Relative intensities of the hot Q branches are compatible with a room temperature Boltzmann distribution of vibrational modes below 200 cm^{-1} such as v_{11} and v_{15} CH$_3$ torsion modes.

A highly diluted jet-cooled laser spectrum of the v_{14} band of DMS (1.5% seeded in 2 bar Ar) was recorded in the 963–987 cm^{-1} range (Fig. 2b) and compared to the room temperature cell-FTIR spectrum (Fig. 2a) which extends between 945 and 1005 cm^{-1}. The drastic reduction of the rovibrational distribution as well as the elimination of hot bands clearly evidences the strong rovibrational cooling of the pulsed supersonic expansion which makes possible an unambiguous band contour analysis. A hotter jet-cooled laser spectrum, more concentrated in DMS (4.5% in 2 bar Ar) has been then recorded to assign more jet-cooled lines in the P branch between 956 and 963 cm^{-1}.

4. Rovibrational analysis and discussion

DMS is a prolate asymmetric top (κ = −0.68) with C_{2v} symmetry at equilibrium and 21 vibrational modes [8]. Any spectroscopic
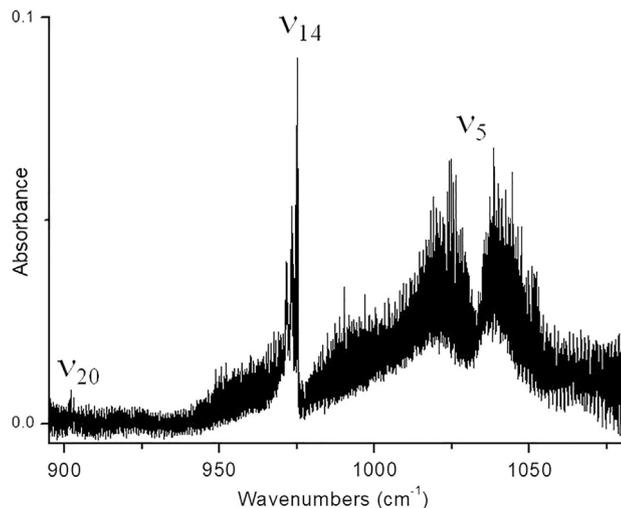
Fig. 1. Cell-FTIR room temperature spectrum of the 9–11 µm region of dimethyl sulfide recorded at 0.003 cm^{-1} resolution.
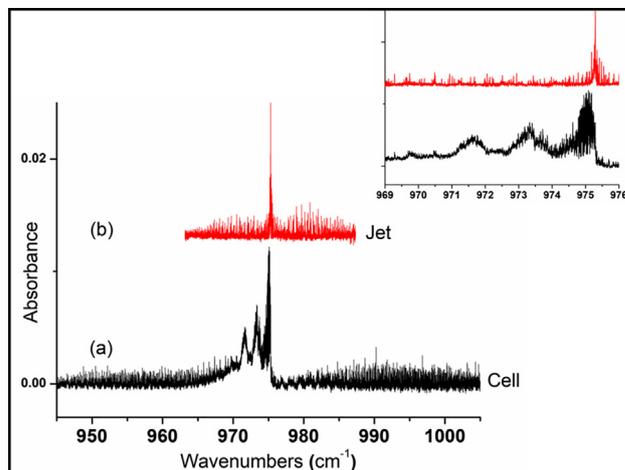
Fig. 2. Comparison between the v$_{14}$ CH$_3$-bending mode spectra of dimethyl sulfide recorded using our jet-cooled EC-QCL spectrometer (a) and cell-FTIR room temperature spectrometer (b). The inset highlights the significant reduction of hot Q branches and the rotational distribution in the jet-cooled spectrum.

study related to this molecule is particularly challenging due to the presence of two equivalent methyl internal rotors with a barrier height for internal rotation of 735.784(44) cm^{-1} [6]. Up to now, only the low frequency v_{15} CH$_3$ torsion mode has been analyzed using high resolution cell-FT spectroscopy and required suitable theoretical models and Hamiltonians to treat the internal rotation splittings. It is expected that such splittings due to large amplitude motion should be too small to be observed in the region of the v_{14}-CH$_3$ bending mode within our experimental resolutions. Consequently, we used the classic Watson's A reduced effective Hamiltonian of a rigid rotor asymmetric top in the I^r representation as described by the following equation:

$$H = [A - \frac{1}{2}(B+C)]\hat{j}_z^2 + \frac{(B+C)}{2}\hat{j}^2 + \frac{1}{2}(B-C)(\hat{j}_x^2 - \hat{j}_y^2) - \Delta_J\hat{j}^4$$
$$- \Delta_{JK}\hat{j}^4\hat{j}_z^2\Delta - _K\hat{j}_z^4 - \delta_K[\hat{j}_z^2,\hat{j}_x^2 - \hat{j}_y^2]_+ - 2\delta_J\hat{j}^2(\hat{j}_x^2 - \hat{j}_y^2)$$

where A, B, C are the rotational constants, Δ_J, Δ_{JK}, Δ_K, δ_J and δ_K are the quartic centrifugal distortion rotational constants.

Preliminary simulations of the v_{14}-CH$_3$ bending mode were carried out using PGOPHER program [25]. The set of starting molecular parameters for ground state are taken from previous microwave and millimeter wave complete study [6] while the band centers were predicted by *ab initio* calculations at the anharmonic CCSD-VTZ level [8].

As a first step, we focused our assignments on the jet-cooled lines originating from P and R branches and we checked our assignments by using ground state combined frequency differences for each rotational series. For K_a values larger than 5, PGOPHER simulation shows that both A$_1$ and A$_2$ components are degenerated which leads to a relatively intense series of lines. This is the case for example of rR5,0(5) and rR5,1(5) transitions (noted also 6$_{60}$ ← 5$_{50}$ and 6$_{61}$ ← 5$_{51}$) on the R branch side, and pP6,0(6) and pP6,1(6) transitions (noted also 5$_{50}$ ← 6$_{60}$ and 5$_{51}$ ← 6$_{61}$) on the P branch side. First assignments for these series of lines are displayed in Fig. 3 and preliminary fits converge quickly to experimental accuracy. Assignments of the other series of rotational lines were iteratively carried out. Fig. 4 displays a first simulation including 522 jet-cooled lines in the 956–987 cm^{-1} range for J and K_a values up to 21 and 14 for the P branch, and up to 14 and 10 for the R branch, respectively. Finally, the jet-cooled spectrum is fitted with a root mean square deviation of 0.00138 cm^{-1}, very close to our estimated experimental accuracy of 0.001 cm^{-1}. Table 1 displays
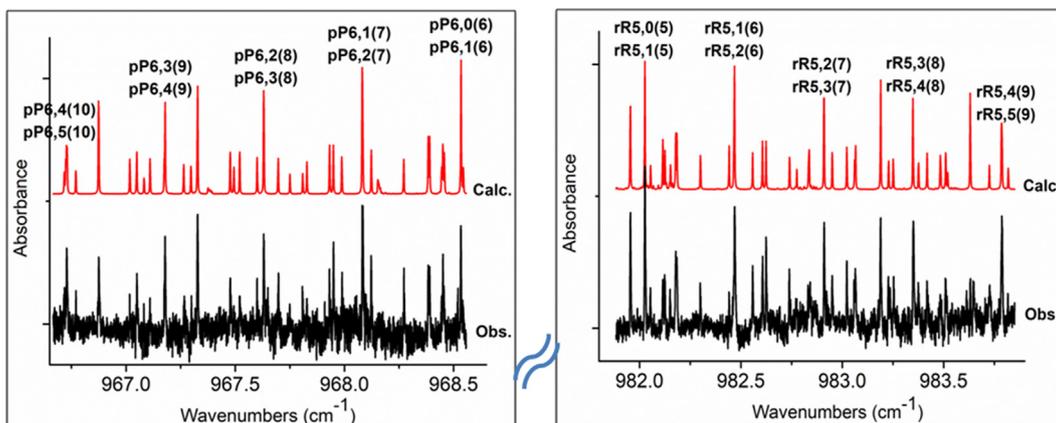
Fig. 3. Comparison between the calculated spectrum at T_R = 20 K and the jet-cooled EC-QCL spectrum in the region of intense pP J = 6, K (J + 4→ J) lines of the P branch and rR J = 5, K (J → J+4) lines of the R branch of the v_{14} CH$_3$-bending mode spectrum of dimethyl sulfide.
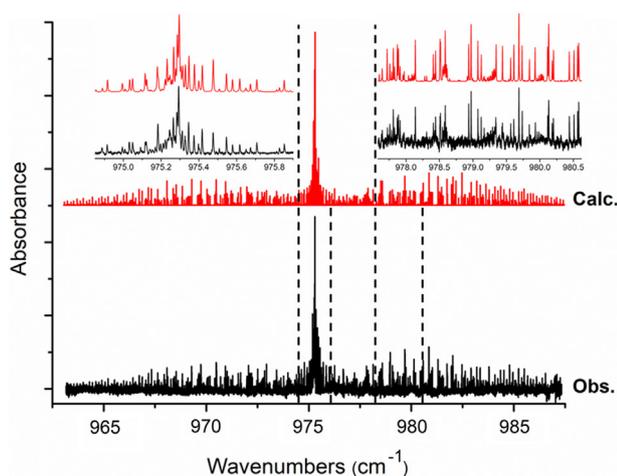
Fig. 4. Comparison between the simulated spectrum at T_R = 20 K of the v_{14} CH$_3$-bending mode of dimethyl sulfide and the jet-cooled EC-QCL spectrum in the 963–987 cm^{-1} range. Two insets of the Q branch and the low J-R branch regions highlight the excellent agreement obtained between observed and calculated spectra from the assignment of 2 jet-cooled lines.

the set 1 of molecular parameters for the v_{14}-CH$_3$ bending mode derived from only the jet-cooled lines. The low rovibrational temperature achieved in the jet spectrum (around 20 K) prevents us to

determine quartic centrifugal distortion rotational constants with a very good precision: higher J and K_a values were required to be introduced in the fitting in order to determine Δ_J, Δ_{JK}, Δ_K, δ_J and δ_K with comparable uncertainties.

In a second step, we analyzed the cell-FTIR spectrum of the v_{14} mode by starting from a prediction of the v_{14} spectrum using set parameters obtained with the jet-cooled lines only (set 1 of Table 1) but calculated at 300 K. With an iterative assignment procedure, we were able to realize a global simulation including 1119 lines (see Appendix A) assigned over the 945–1005 cm^{-1} region (522 jet-cooled and 597 cell lines with root mean square deviations of 0.00138 cm^{-1} and 0.00103 cm^{-1}, respectively) for J and K_a values up to 30 and 23 for the P branch, and up to 29 and 24 for the R branch, respectively. Fig. 5 displays a comparison between room temperature observed and simulated (including the cold fundamental band alone) v_{14} spectra of DMS. The set of molecular parameters derived from the assignment of all jet-cooled and cell lines (set 2) is displayed in Table 1.

In the case of a heavy top asymmetric molecule having three vibrational modes below 300 cm^{-1} such as for DMS, the CSC bending mode (v_7) and the two CH$_3$ torsional modes (v_{11} and v_{15}), a cell spectrum recorded at room temperature alone does not enable to start the rovibrational analysis because of the too strong spectral congestion. The weak intensity of the v_{14} CH$_3$ bending mode required to produce jet-cooled DMS spectra from DMS/Ar mixtures not smaller than 1.5% to obtain a sufficient absorption signal. The relatively high rotational temperature of DMS (about 20 K)

Table 1
Set of molecular parameters of DMS derived for the ground state from a previous microwave and millimeter wave study [6], and for the v_{14}-CH$_3$ bending mode from the present jet-cooled laser and cell-FTIR study.

	Ground state	v_{14}-CH$_3$ bending mode			
		Jet-cooled data (set 1)	% var.[a]	Full data (set 2)	% var.[a]
v_0 (cm^{-1})		975.33527(15)		975.336039(84)	
A (MHz)	17809.72591(81)	17756.85(14)	−0.30	17756.205(28)	−0.30
B (MHz)	7622.12409(52)	7610.578(96)	−0.15	7609.358(67)	−0.17
C (MHz)	5716.74222(58)	5707.659(92)	−0.16	5708.381(82)	−0.15
Δ_J (kHz)	8.0599(63)	8.60(21)	+6.70	8.514(38)	+. 5.63
Δ_{JK} (kHz)	−35.7244(59)	−33.84(78)	−5.27	−36.578(89)	+2.39
Δ_K (kHz)	139.156(65)	133.9(1.1)	−3.78	135.022(92)	−2.97
δ_J (kHz)	2.8339(27)	2.8339[d]		1.333(74)	−52.96
δ_K (kHz)	3.776(42)	3.776[d]		3.776[d]	
N[b]		522		1119	
r.m.s dev. (cm^{-1})[c]		0.0014		0.0014/0.0012	

[a] Variation of spectroscopic parameters in percentage by comparison with those determined in the ground state study [6].
[b] Total number of lines included in the fit.
[c] Root mean square deviation of each set of lines in the fit.
[d] Fixed.
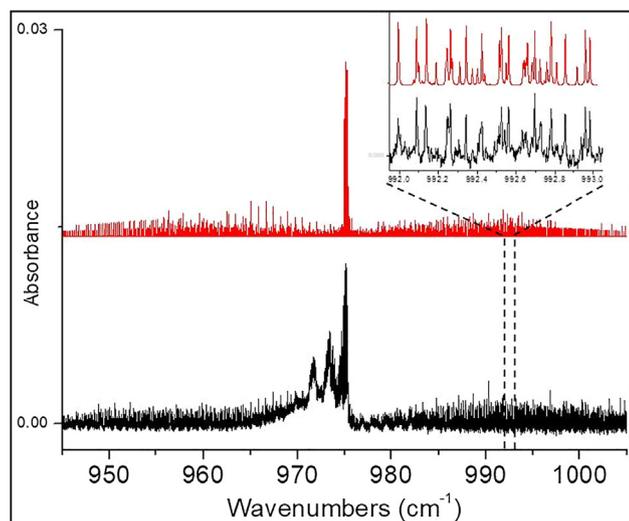
Fig. 5. Comparison between the simulated spectrum at 300 K from the set 2 and the cell spectrum of the v_{14} CH$_3$-bending mode of dimethyl sulfide recorded in the 945–1005 cm^{-1} range. The inset in the 992–993 cm^{-1} range of R branch shows the good match between observed and calculated spectra for most of the intense cell lines. Many weak experimental lines not reproduced by our simulation could be due to P and R branch of hot bands starting from low frequency v_{11} and v_{15} HCH-torsion modes.

achieved in the supersonic expansion compared to a previous jet-cooled study realized with more diluted argon seeded samples (6 K with a mixture of 0.5% CH$_3$ReO$_3$ in 1.2 bar Ar [20]) remain low enough to quench the hot band transitions and keep narrow the rotational distribution.

The parameters derived from the 20 K jet-cooled v_{14} mode of DMS (Table 1) should be considered as a step towards a reliable set of upper state rotational and quartic constants. The 300 K cell spectrum enables to almost double the maximal values of J and K_a reachable and consequently to determine confidently the five upper state quartic constants. The percentage variation of A, B and C for $v_{14} = 1$ with respect to the ground state is very small (about -0.30% in A, -0.17% in B and -0.16% in C), indicating that the mode is almost pure C-H bending added with perhaps a very small S-H displacement. As we can see in Table 1, there is no overlap between the confidence intervals of molecular parameters (within 1σ uncertainty) for jet-cooled and full data set, which clearly proves that the full simulation refines the preliminary jet-cooled data set and enables to determine precisely the δ_J constant in the excited state. Finally, the rigid rotor Hamiltonian used for our analysis is well adapted to our instrumental resolution and allows reproducing the band contour of the v_{14} mode with root mean square deviations very close to experimental accuracies of both laser and FTIR spectrometers.

5. Conclusion

The rovibrational spectrum of the CH$_3$ bending mode of DMS, a sulfur-containing molecule for which substantial attention has been paid in the last decades for the protection of environmental atmosphere was investigated in the atmospheric window around 10 μm. The combination of high resolution FTIR and laser spectroscopic techniques coupled to a pulsed supersonic expansion or a room temperature static absorption cell was successfully used: in a first step the recording of a rovibrationally cold spectrum enables to starting the delicate analysis, in a second step the room temperature cell-FTIR spectrum at 0.003 cm^{-1} resolution is used to refine the upper state molecular parameters up to the quartic ones. Given the resolutions of our Fourier transform and laser spectrometers, we were not able to observe splittings due to internal rotation motion of methyl groups, measured to be on the order of 2 MHz at $J = 10$ in the ground torsional state and 30 MHz at $J = 15$ in the first torsional state [6]. In a near future, QCL Lamb-dip infrared experiments in a room temperature cell at sub-MHz resolution are planned in spectral windows of the v_{14}-CH$_3$ bending mode of DMS free from hot band absorptions in order to investigate internal dynamics in a high frequency vibrational mode.

Appendix A. Supplementary material

Supplementary data associated with this article can be found, in the online version, at https://doi.org/10.1016/j.jms.2018.03.012.

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