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The ν_1 , ν_4 and $3\nu_6$ bands of methyl chloride in the 3.4- μm region: Line positions and intensities

C. Bray^{a,b}, A. Perrin^{c,*}, D. Jacquemart^{a,b}, N. Lacomme^{a,b}^a UPMC Univ Paris 06, Laboratoire de Dynamique, Interactions et Réactivité, UMR 7075, Case Courrier 49, 4 Place Jussieu, 75252 Paris Cedex 05, France^b CNRS, UMR 7075, Laboratoire de Dynamique, Interactions et Réactivité, Case Courrier 49, 4 Place Jussieu, 75252 Paris Cedex 05, France^c Laboratoire Interuniversitaire des Systèmes Atmosphériques, LISA-UMR7583, CNRS and Universités Paris Est Créteil (UPEC) and Paris Diderot-Paris 7, 61 avenue du Général de Gaulle, 94010 Créteil Cedex, France

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ABSTRACT

Methyl chloride (CH₃Cl) is one of the most abundant chlorine-containing molecules in the atmosphere. For this reason a recent update was performed in HITRAN in the 640–2600 cm⁻¹ region based on the line parameters generated in Nikitin et al. [Nikitin A, Champion JP, Bürger H. J Mol Spectrosc 2005;230:174–84] with the intensities scaled to existing experimental data. CH₃Cl has a rather strong signature around 3000 cm⁻¹ which was used recently by the Atmospheric Chemistry Experiment (ACE) satellite mission to produce the first study of the global distribution of methyl chloride in the upper troposphere and stratosphere. However, it was mentioned that the CH₃Cl line positions and intensities spectroscopic parameters are of very low quality in this spectral region in the public access HITRAN or GEISA databases. We present a complete update of the line positions and line intensities for the ν_1 , ν_4 , $3\nu_6$ bands of CH₃³⁵Cl and CH₃³⁷Cl in the 3.4 μm region. For this task, Fourier transform spectra have been recorded at high resolution at the Laboratoire de Dynamique, Interactions et Réactivité in France. Measurements of line positions and line intensities have been retrieved for both isotopologues ¹²CH₃³⁵Cl and ¹²CH₃³⁷Cl in the ν_1 , ν_4 , $3\nu_6$ bands. The theoretical model accounts for the interactions coupling the ($\nu_1=1$; $\ell=0$), ($\nu_4=1$; $\ell=\pm 1$) and ($\nu_6=3$; $\ell=\pm 1$) energy levels, together with additional resonances involving several dark states.

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1. Introduction

One of the most abundant chlorine-containing molecules in the atmosphere is methyl chloride (CH₃Cl), a species whose sources are almost entirely natural. The most common sources of methyl chloride are tropical plants, withering or dead leaves, and biomass burning. As the impacts of the Montreal Protocol and its subsequent amendments are becoming apparent in the reduction of chlorofluorocarbons in the atmosphere, naturally produced methyl chloride is playing an increasingly

significant role in the atmospheric ozone budget. Solar occultation measurements performed from the infrared Fourier transform spectrometer (ACE-FTS) on board the Atmospheric Chemistry Experiment (ACE) satellite mission have been used recently to produce the first study of the global distribution of methyl chloride in the upper troposphere and stratosphere [1]. For this task, the retrievals of CH₃Cl abundances from atmospheric infrared spectra rely on the observation of the Q-branch structures of the ν_1^0 band of CH₃Cl in the 3.4 μm region. The atmospheric retrievals require accurate spectroscopic parameters especially for line positions and intensities.

For the 3.4- μm region, the HITRAN [2] or GEISA [3] linelist for CH₃Cl covers the 2907.8–3182.9 cm⁻¹ region. Fig. 1 gives an overview of the 3.4- μm infrared absorption

* Corresponding author. Tel.: +33 14517 6557; fax: +33 145171564.
E-mail address: Agnes.perrin@lisa.u-pec.fr (A. Perrin).

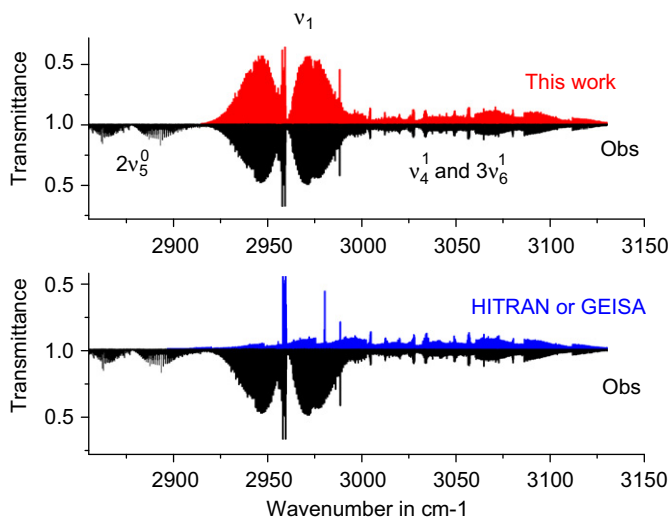


Fig. 1. Overview of the v_1^0 , v_4^1 and $3v_6^1$ band of methyl chloride in the 3.4- μm region. In the 2920–3150 cm^{-1} spectral region, the agreement of the present calculation (upper panel) with the observation (spectrum #3) is significantly improved as compared to the one obtained when using the linelist available in HITRAN [2] or GEISA [3] (lower panel). The present study does not concern the highly perturbed $2v_5^0$ band centered near 2880 cm^{-1} .

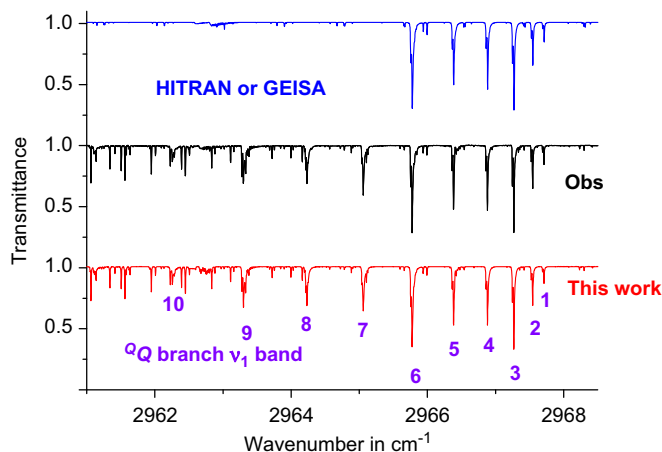


Fig. 2. Part of spectrum #3 near 2965 cm^{-1} . The strong ${}^Q Q_K$ ($\Delta J=0$, $\Delta K=0$) series of the v_1^0 band for $K=1$ to 10 is indicated on the lower trace. All traces have the same vertical scale but are shifted for visual clarity.

region which corresponds to the strong v_1^0 band and to the two times weaker v_4^1 and $3v_6^1$ and $2v_5^0$ bands. The band notation v_4^1 (for example) with $|\ell|$ as superscript corresponds to the vibrational transition between the ($v_4=1$; $\ell=\pm 1$) state and the ground state. Also ℓ refers to $\sum_i \ell_i$, where the ℓ_i are the vibrational angular momentum quantum numbers associated with degenerate modes. As shown in Fig. 2, the most striking deficiencies of the linelist available in the public access databases concern the strong v_1^0 band for which the list is restricted to several ${}^Q Q_K$ structures (for $K=1$ to 6) in the 2965.7–2968.6 cm^{-1} region. Although this list contains numerous lines from the weak v_4^1 and $3v_6^1$ bands, the much stronger P - and R -lines of the v_1^0 band are completely missing, and this is evidenced in Fig. 3 which details a portion of the P -branch of the v_1^0 band.

This is a problem for the atmospheric retrievals performed at 3.4 μm , not only for CH_3Cl , but also for several atmospheric target species, for example ethane (C_2H_6), for which CH_3Cl acts as an interfering molecule at 3.4 μm .

The $\text{CH}_3^{35}\text{Cl}$ and $\text{CH}_3^{37}\text{Cl}$ list present at 3.4 μm in HITRAN [2] or GEISA [3] takes its origin from rather old spectroscopic studies. Only the most recent ones will be mentioned here.

The line positions of the v_1^0 band were investigated by Morillon-Chapey and Graner [4] using grating spectra recorded at medium resolution (0.030 cm^{-1}) and then later by Dang-Nhu et al. [5] by Fourier transform spectroscopy, and no noticeable perturbations were noticed during the v_1^0 band investigation. In Ref. [6], the analysis of the v_4^1 and $3v_6^1$ interfering bands was performed by combining Fourier transform spectra recorded at 0.0074 cm^{-1} resolution with Raman data. Only the strong

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