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Methane line parameters in the HITRAN2012 database



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ABSTRACT

The compilation of methane molecular line parameters was updated to include new global analyses and measurements for $^{12}\text{CH}_4$, $^{13}\text{CH}_4$ and $^{12}\text{CH}_3\text{D}$. Over 70% of the methane parameters in HITRAN2008 were replaced; existing parameters retained were the microwave lines and the Dyad of $^{13}\text{CH}_4$ near $7\ \mu\text{m}$ and ν_6 of $^{13}\text{CH}_3\text{D}$ near $8.7\ \mu\text{m}$, $^{12}\text{CH}_3\text{D}$ ($7\text{--}4076\ \text{cm}^{-1}$), hot bands of $^{12}\text{CH}_4$ ($1887\text{--}3370\ \text{cm}^{-1}$) and normal sample CH_4 ($4800\text{--}5550\ \text{cm}^{-1}$ and $8000\text{--}9200\ \text{cm}^{-1}$). With a minimum intensity at 296 K in units of $\text{cm}^{-1}/(\text{molecule cm}^{-2})$ set to 10^{-37} for the far-IR and 10^{-29} for the mid- and near-IR, the methane database increased from 290,091 lines in HITRAN2008 to 468,013 lines, and three-fourths of these involved the main isotopologue. For $^{12}\text{CH}_4$ and $^{13}\text{CH}_4$, bands from the ground state were revised up to $4800\ \text{cm}^{-1}$. For the first time, $^{13}\text{CH}_4$ and $^{12}\text{CH}_3\text{D}$ line parameters near $2.3\ \mu\text{m}$ were included. Above $5550\ \text{cm}^{-1}$, the new compilation was based on empirical measurements. Prior laboratory results were replaced with extensive new measurements using FTIR ($5550\text{--}5852\ \text{cm}^{-1}$), differential absorption spectroscopy (DAS) and Cavity Ring Down Spectroscopy (CRDS) ($5852\text{--}7912\ \text{cm}^{-1}$). Ground state J values for nearly half of the measured lines in this range were obtained, either by confirming quantum assignments of analyses or by using spectra at 80 and 296 K. Finally, over 11,000

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measured positions, intensities and empirical lower state energies (obtained using cold CH₄) were also added for the first time between 10,923 and 11,502 cm⁻¹. Available pressure broadening measurements from HITRAN2008 were transferred into the new compilation, but 99% of the lines were given crudely-estimated coefficients. New measured intensities and broadening coefficients were included for far-IR transitions, and high accuracy line positions were inserted for the stronger P, Q and R branch transitions of ν_3 at 3.3 μm and $2\nu_3$ at 1.66 μm .

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1. Introduction

Complete and accurate spectroscopy of methane is required for remote sensing of gaseous atmospheres. The various methane-containing targets in the universe involve a wide range of atmospheric temperatures, from less than 50 K for outer planets and their moons to more than 3000 K for exoplanets; thus the temperature dependence of spectroscopic features is crucial. Different astronomical atmospheres are mixtures of methane with other dominant species (air, N₂, H₂, He, etc.) so that reliable pressure-broadened line-shape information is very important. Table 1 lists an overview of what would be needed to provide the ideal methane compilation for universal remote sensing. Traditionally, the HITRAN database was focused on the needs of the Earth observations and only recently were the more extensive spectroscopic requirements of the outer planets considered. The newest HITRAN edition for methane greatly expands the information required for the cold and cooler planets (< 350 K) in terms of the completeness of the database, but future research is needed to support evolving exoplanet studies [1]. In addition, the Earth atmospheric applications now request better accuracy (sub-1%) [2] for the intensities and broadening parameters of stronger transitions in important regions; this will in turn require extensive future studies with non-Voigt line profiles (line mixing, speed dependence, collisional narrowing).

Remote sensing requires compilations that are sufficiently complete and accurate to meet the needs of specific applications. The far- and mid-IR methane spectra are better characterized by theoretical models for the transitions

arising from the ground state and nine hot bands (whose transitions lie between 9 and 10 μm), but at shorter wavelengths, theoretical analyses become difficult because the number of interacting states increases very rapidly. This is seen in Fig. 1 where the vibrational states of methane are plotted in different colors. Quantum mechanical studies can provide the parameters to compute methane features in planetary spectra (purple) up to ~ 6200 cm⁻¹; however, for Earth studies, the predictions above 4800 cm⁻¹ are not yet sufficiently accurate. Above 6200 cm⁻¹ astronomers often resort to low resolution absorption cross sections (red) at shorter wavelengths [3].

To have a complete database for these applications, it is essential that very detailed and complete theoretical models be implemented to predict line positions, intensities, lower state energies and broadening coefficients within the desired accuracies. Extensive measurements are needed to produce and validate such calculations because the fitted constants of effective polyad Hamiltonians and dipole transition moments must be obtained by modeling the experimental data. Line-by-line assignment and fits of experimental spectra are tedious and difficult tasks that can only progress slowly by considering one polyad after the other, in increasing order of energy. Significant progress has been realized recently for ¹²CH₄ [4–6], and in a more limited manner for ¹³CH₄ [7,8]. As discussed later, useful initial values of the model parameters can be estimated by the *ab initio* and effective Hamiltonian approaches to facilitate interpretation of the higher polyads; such an approach with a subsequent empirical optimization permitted new assignments in ¹³CH₄ spectra [7]. In turn, new fitted parameters could

Table 1

Overview of database requirements for remote sensing of methane.

	Earth Very accurate	Outer planets ←In between→	Exoplanets etc. Very complete
Wavelength range (μm)	1.3–9	0.6–500	0.6–9
Temperature range (K)	180–350	40–200	300–3000
Minimum intensity ^a	10 ⁻²⁶	10 ⁻²⁹	??
Number of lines needed	~0.5 Million	10 Million	> 1 Billion
Pressure broadening species	N ₂ , O ₂ , H ₂ O	H ₂ , He, N ₂	H ₂ , N ₂ ?
Accuracies needed			
Positions (in cm ⁻¹) ^b	0.0001	0.001–0.100	0.002–5
Intensities (%)	0.5–3	2–5	10–20
Line shapes (%) ^c	0.5–3 Non-Voigt	2–5 Non-Voigt	10–20 Voigt

^a In cm⁻¹/(molecule cm⁻²) at 296 K.

^b In high pressure atmospheres, accurate pressure shifts are required as well.

^c Line shapes: Lorentz, speed dependence, collisional narrowing and/or line mixing.

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