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Short note

Temperature and pressure dependence of the line shape at $\lambda = 763$ nm in oxygen concentration detection

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ABSTRACT

Gas line shape is determined by the Voigt profile, which is the convolution of Lorentz and Doppler profiles. The calculation amount in the Voigt profile is much larger than that in the two other profiles, and an approximate Lorentz or Doppler profile is generally used in gas concentration detection via tunable laser absorption spectroscopy. The normalized peak ratio and error function are introduced to compare the approximating effect of the two profiles. The normalized peak ratio value is simulated for Doppler profile and Lorentz profiles over a variable temperature and pressure, respectively. The 10%, 5% and 2.5% error functions for pressure versus temperature are obtained for the two profiles. Oxygen at a wavelength of 760 nm is used to demonstrate the simulation results. The presented method of investigating line shapes can be applied to other gas spectrum lines.

1. Introduction

Tunable diode laser absorption spectroscopy (TDLAS) is widely used for gas detection in various industrial, safety and environmental monitoring applications due to its excellent tunability, compactness and low cost [1–8]. Gas line shape is a key factor in TDLAS because it can affect the spectral distribution of the detected signal. Line type is affected by various broadening mechanisms, the most important of which is Doppler and collision broadenings (described by Doppler and Lorentz profiles, respectively) [9–11]. The gas line shape Voigt profile is a convolution of the two other profiles. However, the Voigt profile often entails a large amount of calculation. A reasonable approximation must be made under appropriate conditions. Under high-pressure conditions, the Lorentz profile dominates the gas line shape, and the Doppler profile dominates the gas line shape under high-temperature and low-pressure conditions.

Oxygen concentration monitoring has elicited much attention [12–17] due to its importance in combustion applications, energy studies, atmosphere security control, and food and drug production control. In this work, we investigate the line shape of oxygen at a wavelength of 760 nm over various temperature and pressure.

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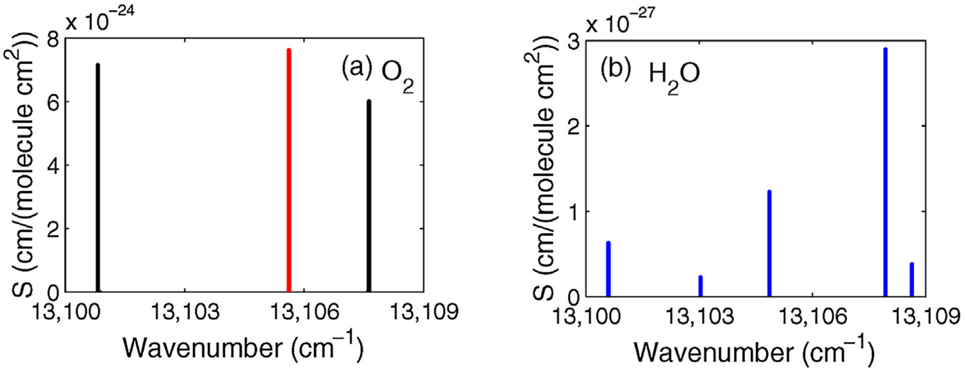

Fig. 1. Absorption spectrum of (a) O_2 and (b) H_2O molecular around 763 nm.

2. Characteristics of spectral line and theory

2.1. O_2 absorption characteristics around 763 nm

According to the HITRAN database [18], O_2 has a strong isolated absorption line around the wavelength of 763 nm (corresponding to 13105.6 cm^{-1}), and other lines are far from this line (Fig. 1(a)). Compared with other important absorption gases, H_2O has a much weaker spectrum at 763 nm (Fig. 1(b)). At a certain pressure and temperature variation range, the halfwidth at half maximum (HWHM) is much smaller than the interval between lines. Therefore, the isolated line at 763 nm can be used to study the variation in gas line over pressure and temperature without being affected by other lines.

2.2. Theory

2.2.1. Doppler profile

The Doppler profile can be expressed by a Gaussian function as [19]

$$\Psi\left(\nu, T\right) = \frac{1}{\alpha_D(T)}\sqrt{\frac{\ln 2}{\pi}}\exp\left[-\ln 2\left(\frac{\nu-\nu_c}{\alpha_D(T)}\right)^2\right], \quad (1)$$

where T is environment temperature, ν is frequency, ν_c is the frequency in the gas spectral line center, and $\alpha_D(T)$ is the halfwidth (HWHM) of the Gaussian function, which can be expressed as

$$\alpha_D(T) = \frac{\nu_c}{c}\sqrt{\frac{2\ln 2N_A kT}{m}}, \quad (2)$$

where c is the speed of light, N_A is the Avogadro constant, k is the Boltzmann constant, and m is the oxygen molecular mass.

2.2.2. Lorentz profile

For oxygen at total pressure p, temperature T, and oxygen partial pressure p_s, the halfwidth of the Lorentz profile $\alpha_L(p, p_s, T)$ can be calculated as [20]

$$\alpha_L(p, p_s, T) = \left(\frac{T_{\rm ref}}{T}\right)^n((\alpha_{\rm air}(p_{\rm ref}, T_{\rm ref})(p-p_s) + \alpha_{\rm self}(p_{\rm ref}, T_{\rm ref})p_s), \quad (3)$$

where α_{air} and α_{self} are the air-broadened and self-broadened halfwidths, respectively, at T_{ref} = 296 K and reference pressure p_{ref} = 1 atm. The values of α_{air} and α_{self} are relatively close, they are 0.053 and 0.052 cm^{-1}, respectively. Ignoring the influence of p_s, Eq. (3) can be expressed as

$$\alpha_L(p, T) = \left(\frac{T_{\rm ref}}{T}\right)^n(\alpha_{\rm air}p_{\rm ref}, T_{\rm ref})p. \quad (4)$$

The pressure shift of the line center frequency leads to a shifted frequency ν_{cp} given by

$$\nu_{\rm cp}(p) = \nu_c + \delta(p_{\rm ref})p, \quad (5)$$

where δ is the pressure shift of the line.

The Lorentz profile is given by

$$\Psi_L(\nu, p, T) = \frac{1}{\pi}\frac{\alpha_L(p, T)}{\alpha_L(p, T)^2 + (\nu - \nu_{\rm cp}(p))^2} \quad (6)$$