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Temperature dependent pressure induced linewidths of $^{16}O_2$ and $^{18}O^{16}O$ transitions in nitrogen, oxygen and air

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Abstract

The temperature dependent pressure induced broadening of several oxygen resonant transitions have been measured. For $^{16}O_2$ the isolated magnetic fine-structure transition $J'_{N'} \leftarrow J_N = 1_1 \leftarrow 1_0$ and the magnetic rotational transition $3_2 \leftarrow 1_2$ are investigated in both nitrogen and oxygen. Additionally, pressure broadening of the magnetic rotational transition of $^{18}O^{16}O$ $2_1 \leftarrow 0_1$ is measured in air. This work improves precision and accuracy of the linewidth of the fine-structure transition and provides the first temperature dependent linewidth measurements at higher frequency.

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1. Introduction

By virtue of a fixed mixing ratio, remote sensing of molecular oxygen resonances in the earth atmosphere affords determination of either vertical temperature profiles or pointing accuracy or both. In order to extract such information from remote sensing data detailed knowledge of the molecular spectroscopy is required. The magnetic dipole moment of two Bohr magnetons determines the intensities of the magnetic rotational and fine-structure resonant transitions. The molecular Hamiltonians of $^{16}O_2$ [1] and $^{18}O^{16}O$ [2] provide necessary information on transition frequency, Doppler width and intensity temperature dependence. In a relatively dense gas, such as the earth atmosphere, the collision-induced linewidth is also of importance. Well-founded theoretical predictions of collision-induced linewidths and their temperature dependence require extensive calculation of inter-molecular potential dynamics. For oxygen, inter-molecular potentials are available and calculations have been done for many transitions [3]. Nevertheless, even well-founded calculations often differ from quantitative experimental measurements by several percent. Consequently, many experimental studies have been performed to measure pressure broadening of oxygen in buffer gases of nitrogen, oxygen, or air [1,4–19].

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The Earth Observing System Microwave Limb Sounder (EOS-MLS) [20] currently observes both the $1_1 \leftarrow 1_0$ $^{16}O_2$ transition at 118.75 GHz and the $2_1 \leftarrow 0_1$ $^{18}O^{16}O$ transition at 233.95 GHz. For proper inversion of the radiance signatures the parameters of the pressure broadening relationship shown in the following equation are required:

$$\Gamma(T,p) = \gamma_o p \left(\frac{296}{T}\right)^n. \qquad (1)$$

Eq. (1) is the phenomenological power law description of temperature dependent collisional broadening in which the Lorentzian width $\Gamma(T,p)$ is described by the width at a reference temperature and pressure, $\gamma_o = \Gamma(296\,\mathrm{K}, 1\,\mathrm{Torr})$, which is then parameterized by the exponent, n to give a smooth temperature dependence. Tabulation of these parameters in the HITRAN [21] database is based upon the (calculated air) broadening data from Brown and Plymate [22] which includes an aggregate temperature dependence of all transitions, $n = 0.71$. However, these data have not directly agreed with rotational studies. An extensive survey of $^{16}O_2$ pressure broadening in N_2 and O_2 at room temperature [1] shows a systematic increase of 15% from the values listed in HITRAN. Only a few sources [9,14,19] of reduced temperature measurements are available for pure rotational transitions of $^{16}O_2$. Refs. [9] and [14] suggest higher values for n as compared to HITRAN, whereas the recent work of Tretyakov et al. [19] is in agreement with the HITRAN adopted value. No previous laboratory measurements of broadening for rotational transitions of $^{18}O^{16}O$ are known. Consequently, the required data for thorough analysis of the EOS-MLS profiles is incomplete and the present study was conducted to meet the mission needs.

2. Experimental

Measurements were carried out with two similar free-space cells; $L = 1.0$ and 0.7 m, with 5.0 and 7.3 cm diameters, respectively. The 1.0-m length cell was designed for static gas measurements whereas the 0.7 m cell is of the traditional flow design [23]. The static cell and general experimental setup are shown in Fig. 1. Each cell is enclosed within a temperature controlled jacket, shown by the gray area in the figure. For reduced

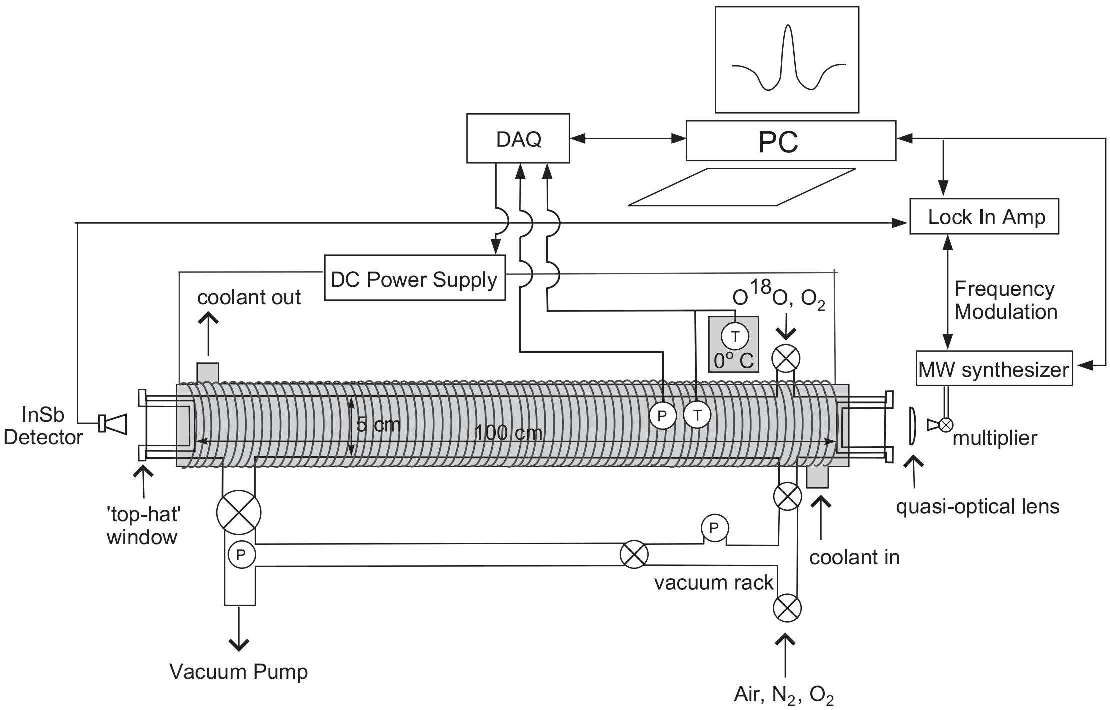

Fig. 1. Experimental setup for measurement of oxygen lineshapes. Pressure gauges are labeled as Ⓟ and thermocouples Ⓣ.