

Shape of the 5 mm Oxygen Band in the Atmosphere

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Abstract—The problem of absorption of microwaves by molecular oxygen in the atmosphere is treated by means of a first-order approximation to the impact theory of overlapping spectral lines. By including only the coupling between adjacent rotational states in molecular collisions, we have devised a simple approximate method for computing the interference between lines from measurements on the resolved lines. The need for an empirically determined function describing the linewidth/pressure ratio is eliminated. Comparisons with measurements at atmospheric pressures show that the first-order interference accounts for the low absorption at the band wings near 1 atm pressure. It also predicts the correct amount of asymmetry between high and low frequency wings. Improvement over previous models for the pressure broadening is obtained at frequencies $\gtrsim 55$ GHz. This approach is not specific to oxygen and could be adapted to other similar molecules.

I. INTRODUCTION

THE ABSORPTION of millimeter waves by atmospheric oxygen is of interest in many fields. Use of the strong absorption region near 5 mm for remote sensing of the atmospheric temperature profile was first proposed by Meeks and Lilley [1]. A successful remote sensing experiment employing a microwave spectrometer has recently been flown on the Nimbus 5 satellite [2]. Attenuation in the window regions of the spectrum due to the wings of the 5 mm band is of interest in the fields of radio astronomy and communications [3]. For these and for other studies of microwave propagation in the atmosphere there is a need for expressions for the absorption coefficient due to oxygen as a function of frequency, pressure, and temperature. These expressions should be accurate but must not involve prohibitive amounts of computation.

The theory of bands composed of overlapping lines has been developed by many authors, notably Baranger [4], Kolb and Griem [5], and Gordon [6], [7]. Gordon's formulation is useful for our purpose since it allows a semiclassical interpretation of the molecular collision process. Computation of the collision cross section matrix that determines interference (or blending) of the lines requires an integration over all possible trajectories however, and the result depends on temperature. Computations of the pressure broadened spectrum of oxygen have been carried out in [8]–[11]. The complexity of these computations has heretofore prevented application of the theory of overlapping lines to the practical problem of atmospheric absorption, however.

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Previously, the solution to this problem has been to sum lineshapes derived for isolated lines. The ratio linewidth/pressure, which would be constant for an isolated line, was reduced with increasing pressure to fit measurements of total absorption, particularly in the band wings. This is the procedure followed in [1], [12], and [13], where the Van Vleck–Weisskopf [14] lineshape was used, and in [15] where the Gross [16] or Zhevakin–Naumov [17] lineshape was used. The linewidth correction at 1 atm amounted to a factor of 2 to 3, depending on the model. This procedure is not entirely satisfactory because the functional form chosen to make the fit is ad hoc; thus there is a risk of erroneous results in regions of frequency-pressure-temperature space for which data is unavailable at the time the fitting is done.

The procedure that will be developed in this paper involves two approximations. The first is a scheme for determining the largest of the matrix elements that govern line interference, from measurements of resolved linewidths. The general principles of detailed balance and conservation of probability are utilized. This approximation should be valid when rotational states are weakly coupled by collisions. Secondly, to eliminate matrix operations the band shape is expanded to first order in pressure.

II. FORMULATION

A. The Oxygen Spectrum

Van Vleck [18] has described the basic characteristics of the spectrum of molecular oxygen $^{16}\text{O}_2$ in its ground state. Only odd values of the rotational quantum number N are allowed. Coupling of electronic spin with rotational angular momentum forms a triplet of states with total angular momentum $J = N - 1$, N , or $N + 1$. The level $J = N$ is highest in energy. Selection rules permit two types of magnetic dipole transitions. Transitions between the state $J = N$ and the state $J = N \pm 1$ give rise to resonant absorption at frequencies ν_N^\pm , listed in Table I for $N \leq 39$. Nonresonant absorption results from interactions with the states $J = N \pm 1$ in which $\Delta J = 0$.

In this paper we will be concerned with the pressure range 1 to 1000 mbar. In this range collisions between molecules are the dominant line broadening mechanism. The absorption coefficient γ may be expressed as

$$\gamma = CP[\nu/T]^2 F. \quad (1)$$

When temperature T is given in K, pressure P in mbar and frequency ν in GHz, the constant C is equal to 0.330 for γ in Np/km or 1.434 for γ in dB/km. The function F together with the factor ν^2 determines the band shape.