LINE INTENSITY MEASUREMENTS AND FAR-WING INTENSITY REDISTRIBUTION IN THE 0.76 μM O_2 BAND

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Molecular oxygen (O_2) has a well-known and uniform molar fraction within Earth's atmosphere. Because of this, the near-infrared O_2 molecular absorption bands, centered at 0.76 μm and 1.27 μm, are commonly used in remote sensing (TCCON, COCCON) and satellite missions (GOSAT, OCO-2/3, SCIAMACHY) to measure atmospheric air mass. For these missions, physics-based spectroscopic models and experimentally and theoretically determined line-by-line parameters are used to predict the temperature- and pressure-dependence of the absorption cross-section as a function of wave number, pressure, temperature, and water vapor concentration. The accuracy of atmospheric retrievals requires the spectroscopic model to describe all relevant physics. The Hartmann-Tran line profile is recommended for high-resolution spectroscopy and can be reduced to the well-known Voigt profile [1]. This profile assumes that collisions occur instantaneously. However, when this assumption is not satisfied, the finite duration of collisions leads to a redistribution of the line intensity from the line cores to the far wings, an effect that increases with pressure [2-4]. Failure to account for this redistribution leads to an apparent depletion in the core line intensity as a function of pressure, such that retrieved concentration would yield a bias if determined from absorption cross-section based on observations acquired at substantially different pressures. This work reports cavity ring-down spectroscopy measurements of line intensities and pressure-dependent intensity redistribution in the 0.76 μm O_2 band. The core intensity depletion magnitude and rotational quantum number dependence are compared to those calculated by renormalized classical molecular dynamic simulations. Additionally, we discuss how including the previously unaccounted-for physics might affect satellite and remote sensing retrievals.

[1] Tennyson, J., et al., Pure and Applied Chemistry, 2014. 86(12): p. 1931-1943. [2] Reed, Z.D., et al., Phys Rev Lett, 2023. 130(14): p. 143001. [3] Tran, H., et al., J Chem Phys, 2023. 158(18). [4] Tran, H., et al., Phys Chem Chem Phys, 2023. 25(15): p. 10343-10352.