

EXTENSIVE INVESTIGATION OF ROOM-TEMPERATURE CH₃C¹⁴N-N₂ PRESSURE-BROADENING PARAMETERS IN THE 180–1400 GHz RANGE

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Acetonitrile CH₃CN is a molecule of atmospheric interest, now included in the HITRAN database [1]. However, except for some experimental studies of line intensities, positions, broadening and shifting parameters [2,3], its line broadening by many atmospheric gases remains incomplete. The case of N₂-broadening is the most important since nitrogen is the main perturbing gas in the atmospheres of Earth and Titan. In the present work we address N₂-broadening coefficients of CH₃C¹⁴N rotational transitions for a wide range of rotational quantum numbers J and K .

Experiments were performed with a frequency-modulated spectrometer operating in the 180–1400 GHz range and consisting of a 10–20 GHz frequency synthesizer followed by a frequency multiplier chain based on solid-state devices, a 1.1 meter long absorption inox cell and a bolometric detection. Measurements were done at room temperature, with the active-gas pressure equal to 2–5 mTorr and the buffer-gas pressure 50–600 mTorr. Rotational lines with $J = 9, 12, 15, 21, 27, 33, 42, 48, 63, 69, 75$ and $K \leq 15$, located in the region 184–1390 GHz, have been studied in detail. All recorded lines exhibit clear departures from the usual Voigt profile and have been analyzed using the more realistic Speed-Dependent Voigt profile. The Voigt profile has been also employed because of its continuing use in atmospheric applications.

Measured values are compared to theoretical estimates obtained by the semi-empirical method [4] successfully applied previously to other symmetric tops CH₃X [5] and well appropriate for the CH₃CN-N₂ case because of strong electrostatic interactions due to the large dipole moment of the absorbing molecule. Being fitted on experimental J - and K -dependent values of pressure-broadening coefficients, the theoretical model parameters enable computations of line-shape parameters for enlarged ranges of rotational quantum numbers.

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[3] J.-M. Colmont et al., J. Mol. Spectrosc. 238, 98 (2006).

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