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Title:Experimental studies by complementary terahertz techniques and semi-classical calculations of N2- broadening coefficients of CH335Cl
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Abstract:Room-temperature N<inf>2</inf>-broadening coefficients of methyl chloride rotational lines are measured over a large interval of quantum numbers (6≤J≤50, 0≤K≤18) by a submillimeter frequency-multiplication chain (J≤31) and a terahertz photomixing continuous-wave spectrometer (J≥31). In order to check the accuracy of both techniques, the measurements of identical lines are compared for J=31. The pressure broadening coefficients are deduced from line fits using mainly a Voigt profile model. The excellent signal-to-noise ratio of the frequency-multiplication scheme highlights some speed dependence effect on the line shape. Theoretical values of these coefficients are calculated by a semi-classical approach with exact trajectories. An intermolecular potential including atom-atom interactions is used for the first time. It is shown that, contrary to the previous theoretical predictions, the contributions of short-range forces are important for all values of the rotational quantum numbers. Additional testing of modifications required in the semi-classical formalism for a correct application of the cumulant expansion is also performed. It is stated that the use of the cumulant average on the rotational states of the perturbing molecule leads, for high J and small K values, to slightly higher line-broadening coefficients, as expected for the relatively strong interacting CH<inf>3</inf>Cl-N<inf>2</inf> system. The excellent agreement between the theoretical and the experimental results ensures the reliability of these data. © 2012 Elsevier Ltd.
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