# Temperature dependence of $CH_3{}^{35}Cl$ and $CH_3{}^{37}Cl$ air-broadening coefficients by a semi-classical approach

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Methyl chloride $CH_3Cl$ is known as the main source of chlorine ions in the Earth's atmosphere. These ions are important catalysts of chemical reactions leading to the depletion of the stratospheric ozone layer. As a consequence, a precise knowledge of $CH_3Cl$ line widths and shifts due to the main atmospheric perturbers $N_2$ and $O_2$ is of a crucial importance for atmospheric studies. These data are required for various spectral regions (various bands) and for wide temperature ranges. Unfortunately, no direct air-broadening measurements have been performed up to now even at room temperature and the detailed information about the temperature-dependence of air-broadening and shifting $CH_3Cl$ coefficients is missing in main spectroscopic databases.

The present work reports air-broadening coefficients at 296 K and corresponding temperature-dependence exponents semi-classically calculated for $CH_3{}^{35}Cl$ and $CH_3{}^{37}Cl$ (vib)rotational transitions ($0 \le J \le 70$, $0 \le K \le 20$) in order to provide the required data.

In contrast with previous calculations by other authors, the active molecule is rigorously treated as a symmetric top, long- as well as short-range interactions are accounted for, and exact classical trajectories are employed to describe the relative motion of colliders. This approach, already validated on extensive room-temperature measurements for the $CH_3{}^{35}Cl$-$O_2$ and $CH_3{}^{35}Cl$-$N_2$ systems [1–3], yields quite realistic estimations of $N_2$- and $O_2$- broadening temperature exponents, so that line widths calculated for 203 K compare very favorably with available experimental data [4]. Successful testing on $N_2$- and $O_2$-broadening data ensures the reliability of the reported values for $CH_3Cl$-air in the interval of atmospheric interest 200–300 K [5].

[1] J. Buldyreva, M. Guinet, S. Eliet, F. Hindle, G. Mouret, R. Bocquet, A. Cuisset, *PCCP* **2011**, *13*, 20326.
[2] M. Guinet, F. Rohart, J. Buldyreva, V. Gupta, S. Eliet, R.A. Motiyenko, L. Margulès, A. Cuisset, F. Hindle, G. Mouret, *JQSRT* **2012**, *113*, 1113.
[3] C. Bray, D. Jacquemart, J. Buldyreva, N. Lacome, A. Perrin, *JQSRT* **2012**, *113*, 1102.
[4] J.-P. Bouanich, G. Blanquet, J.-C. Populaire, J. Walrand, *J. Mol. Spectrosc.* **2001**, *208*, 72.
[5] J. Buldyreva, *JQSRT* **2013** (in press); DOI : 10.1016/j.jqsrt.2013.04.003.