SEMICLASSICAL ESTIMATES OF PRESSURE-INDUCED LINE-WIDTHS FOR INFRARED ABSORPTION BY EXOMOLECULES

K. STEHLIN[*], **J. BULDYREVA**[*], **S.N. YURCHENKO**[*,**], **J. TENNYSON**[**],
Institut UTINAM, UMR CNRS 6213, Université de Franche-Comté, 16 route de Gray, 25030 Besançon cedex, France (*); Department of Physics and Astronomy, University College London, Gower Street, WC1E 6BT London, United Kingdom (**)

Molecules and molecular ions found or expected in exoplanetary atmospheres are generally poorly characterized from the viewpoint of their spectroscopic line-shape parameters; in many cases, there are no data at all. From the experimental point of view, this fact is due to elevated temperatures and high fluxes of stellar radiation irreproducible in laboratory conditions. From the theoretical point of view, potential energy surfaces for required molecular pairs are unavailable and advanced (computationally expensive) calculations can not be performed.

As account for and completeness of such data are crucial for reliable simulations of radiative transfer in the atmospheres of exoplanets [1], we employ a simple semi-classical expression [2] to generate rotationally-independent estimates of pressure-broadened linewiths for (vib)rotational transitions. A wide range of absorbers and perturbation including He, Ar, H_2, N_2, O_2, CO, NO, CO_2, H_2O, CH_4, NH_3 and self-perturbation are considered. The leading long-range interaction term, molecular masses and kinetic diameters as well as temperature are used as input parameters, allowing tables of pressure-broadening coefficients $\gamma(T_{\rm ref})$ at the reference temperature $T_{\rm ref}$=296 K to be produced. Values $\gamma(T)$ for other temperatures T can be readily obtained using the power law $\gamma(T) = \gamma(T_{\rm ref})(T_{\rm ref}/T)^{0.5}$. In some cases kinetic diameters were unavailable but Lennard-Jones parameters σ could be found and were used instead. For most cases none of them were found, and the required kinetic diameters were estimated by a semi-empirical formula [3] from the molecular polarizabilities.

These theoretical estimates provide data on collision pairs which are so far completely missing in spectroscopic databases. They should prove useful for remote sensing of exoplanetary atmospheres.

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[1] J.J. Fortney et al., arXiv:1905.07064 (2019).
[2] J. Buldyreva et al., *RASTI*, **1**, 43 (2022), doi:10.1093/rasti/rzac004.
[3] B.I. Loukhovitski and A.S. Sharipov, *J. Phys. Chem. A*, **125**, 5117 (2021), doi:10.1021/acs.jpca.1c02201.