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# THE IMPACT OF NEW COLLISIONAL RATES ON THE WATER EMISSION

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**Abstract.**
The interpretation of water emission from current observations and future Herschel/HIFI data requires a detailed knowledge of collisional rate coefficients. The rotational (de)excitation of $H_2O$ by $H_2$ molecules is one of the most relevant collisional processes in interstellar and circumstellar media. We have recently computed quasi-classical rate coefficients for all transitions among the lowest 45 para and 45 ortho rotational levels of $H_2O$ colliding with both para and ortho $H_2$ in the temperature range 20−2000 K. By comparison with quantum calculations, classical rates are found to be accurate within a factor of 1−3 for the dominant transitions. Large velocity gradient modelling shows that these new rates have a significant impact on water emission line fluxes.

## 1 Introduction

Water is ubiquitous in space. Observing and measuring the water lines and its abundance are among the major drives of the high resolution spectrometer *Heterodyne Instrument for the Far Infrared* (HIFI) on board the ESA funded Herschel satellite, which will be launched in 2008. It is however largely recognized by the astronomical community that little new information will be obtained if collisional rates adapted to a wide range of physical conditions are not available. In interstellar and circumstellar regions, $H_2$ is in general the dominant form of hydrogen and the main exciting partner. Quantum calculations of rates for excitation by $H_2$ are however computationally very expensive and the present work was motivated by the possibility of performing quasi-classical trajectory (QCT) calculations as a cheap alternative. We report below large velocity gradient (LVG) calculations based on classical rates whose impact on water line fluxes is illustrated.

## 2 Method

Quantum and QCT collisional calculations were performed with rigid molecules using the $H_2O-H_2$ vibrationally averaged potential energy surface of Faure et al. (2005). Full details on the quantum and classical calculations can be found in Dubernet et al. (2006) and Faure et al. (2007), respectively. For the astrophyscal modelling, we employed a LVG code that refers to a semi-infinite isodense and isothermal slab (plane-parallel geometry). It solves self-consistently the statistical level populations and the radiative transfer equations under the approximation of the escape probability, assuming a gradient in the velocity field. The computed line spectrum depends on a few basic parameters: the density of the colliders ($n_{H_2}$), the temperature of the emitting gas ($T$), the water column density ($N_{H_2O}$) and the maximum gas velocity (here 1 km/s). We consider in the following the case of optically thick lines: $N_{H_2O}=10^{15}$ cm$^{-2}$. The pumping of the levels by infrared and submillimetre radiation is neglected in order to focus on the impact of collisions. In this context it should be noted that even in the case of strongly optically thick lines, the lines can be "effectively optically thin" if the levels are very sub-thermally populated, as is often the case for water lines.

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## 3 Results

In Fig. 1, two sets of rate coefficients for rotational de-excitation of the ortho-$H_2O$ $3_{03}$ level by para-$H_2$ are plotted as a function of temperature: the present QCT data between 50 and 2000 K, and the quantum data of Dubernet et al. (2006) at 20 K augmented with unpublished quantum data between 20 and 1500 K. It can be observed that there is an overall good agreement between the classical and the quantum data. The agreement is even excellent above 100 K where quantum data are within the error bars of the QCT data. At and below 100 K, the agreement is not as good, reflecting the limitations of the classical approach (see Faure et al. 2007), but differences do not exceed a factor of 2. We note that a good agreement was also observed with the low temperature $H_2O-H_2$ rates of Phillips et al. (1996). On the other hand, large differences (up to 2 orders of magnitude) were found with the scaled $H_2O-He$ rates of Green et al. (1993).

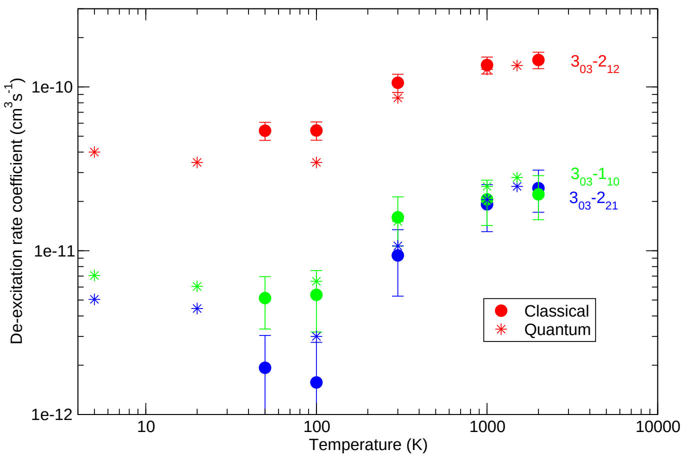


**Fig. 1.** Rate coefficients for rotational de-excitation of the ortho-$H_2O$ state $3_{03}$ by para-$H_2$ as a function of temperature. Stars denote the quantum results while circles with error bars (two standard deviations) give the QCT results.

Three sets of collisional data were employed: the scaled $H_2O$-He rates of Green et al. (1993), the $H_2O-H_2$ rates of Phillips et al. (1996) and the newly calculated $H_2O-H_2$ classical rates of Faure et al. (2007). Line flux ratios for para-$H_2O$ transitions at a representative set of density and temperature are reported in Fig. 1. Collision rates with ortho-$H_2$ only were considered to simplify the interpretation. It can be observed that LVG fluxes based on the classical rates are increased up to a factor of 20 with respect to fluxes based on the scaled $H_2O-He$ rates. On the other hand, LVG fluxes based on the classical rates are very similar to those based on the rates of Phillips et al. (1996), with flux ratios close to 1. These findings reflect the differences in collision rates (see Faure et al. 2007) and show that differences in rates are not amplified within the radiative transfer equations. We also observe that the flux ratios rise steeply with increasing upper energies, as expected from the increase of critical densities.

## 4 Conclusion

New collisional rates for $H_2O-H_2$ calculated at the quasi-classical level (Faure et al. 2007) have been shown to increase the water emission line fluxes by large factors with respect to fluxes based on the (scaled) $H_2O-He$ rates currently used by astronomers. These new rates should therefore be adopted in any detailed population model of water in warm and hot environments. We note, however, that the accuracy of the classical rates is limited by the use of classical mechanics and that accurate quantum rates, currently in progress (Dubernet and co-workers), will ultimately replace the classical rates, except possibly in physical regimes where quantum theory remains prohibitively expensive.

## References

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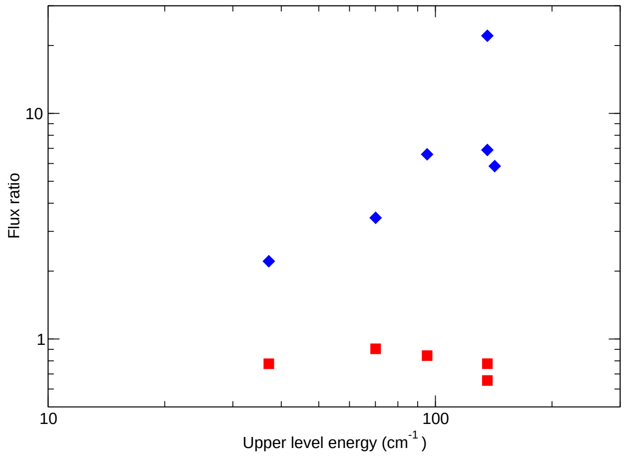


**Fig. 2.** Emission line flux ratios as functions of the upper energy levels of para-$H_2O$ for $n_{H_2} = 10^6$ cm$^{-3}$ and $T = 100$ K. Squares (diamonds) denote the ratios between LVG fluxes based on classical rates and fluxes based on the $H_2O-H_2$ rates of Phillips et al. (1996) (scaled $H_2O-He$ rate of Green et al. 1993). Only transitions whose fluxes are larger than 1% of the total flux are plotted.

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