

# State-to-state cross sections and rate coefficients for the rotational excitation of polyatomic hydrides in astrophysical environments

## Content

Recent astronomical observations have been showed that interstellar molecular clouds exhibit a very rich and complex chemistry [1]. In order to understand in details the chemical composition in such environments, a non-LTE analysis of the emission spectra is necessary. This requires reliable determination of collisional rate coefficients for the transitions between rotational levels of the target molecular species.

Both the isoelectronic hydronium cation ( $\text{H}_3\text{O}^+$ ) [2] and ammonia molecule ( $\text{NH}_3$ ) [3] have been detected in different regions of the interstellar medium (ISM). While  $\text{H}_3\text{O}^+$  plays a crucial role in oxygen and water chemistry in the ISM,  $\text{NH}_3$  has been widely used as a probe of physical conditions in interstellar environments. Thus, studying their collisional excitation is of high importance for the proper interpretation of astrophysical observations.

The rotational excitation of  $\text{H}_3\text{O}^+$  in collision with  $\text{H}_2$  molecule is studied for the first time [4]. State-to-state rotational de-excitation cross sections were computed using the close-coupling method, based on a highly accurate 5D potential energy surface [5]. The thermal rate coefficients were then derived up to 300 K kinetic temperatures.

We also present collisional data obtained for the excitation of  $\text{NH}_3$  by  $\text{H}_2$ . We have noticeably extended the range of collision energies (up to  $4500 \text{ cm}^{-1}$ ) and kinetic temperatures (up to 500 K), compared to previous studies by Bouhafs et al. [6] for this system. A comparative analysis of cross sections and rate coefficients is provided for the  $\text{H}_3\text{O}^+$  and  $\text{NH}_3$  target molecules. The calculated rate coefficients are used for modeling the collisional excitation of these species in interstellar molecular clouds.

## References

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