

# Computational Astrochemistry: H<sub>2</sub>O - H<sub>2</sub> collisions

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Quantum mechanical calculations play an important role in astrochemistry. Excitation of molecules in dense regions of interstellar medium occurs mainly through collisions with abundant species such as H<sub>2</sub> and He. Thus, computation of the collisional rate coefficients are necessary to infer the physico-chemical parameters of the gas. Here, we calculate the inelastic cross sections for the collisions of H<sub>2</sub>O and H<sub>2</sub> including very high rotational levels. These calculations are important to analyze the forthcoming data from the James Webb Space Telescope, which will observe hot H<sub>2</sub>O lines with unprecedented sensitivity.

## 1 Introduction

Star formation occurs deep inside molecular clouds, where temperatures and densities are much higher than in a quiescent interstellar medium ( $T = 30\text{ K}$ ,  $n_{\text{H}} = 100\text{ cm}^{-3}$ ). Energetic processes such as jets and outflows heat up the gas up to temperatures of few thousands K. The only means to constrain the physical parameters and chemical content of those regions are interstellar molecules. In particular, the proper understanding of molecular collisions provide information about the densities and temperatures of the medium. Quantum chemical calculations are the key step to link observations with physical interpretation.

## 2 James Webb Space Telescope

The James Webb Space Telescope (JWST) is the 6.5 m infrared telescope planned to be launched in 2020. The sensitivity of the telescope will allow to detect many new lines in the MIR (5 – 25  $\mu\text{m}$ ). In this range, we expect tens of high-energy H<sub>2</sub>O lines which have been never detected before.

## 3 H<sub>2</sub>O Energy Levels

Water is one of the most abundant molecule which is detected in the space. Depending on the environments it can be created in different reactions, such as neutral-neutral reaction in shocked gas where temperatures are quite high ( $> 300\text{ K}$ ) or on the grains due to collisions between atoms and subsequent evaporation (van Dishoeck et al., 2013). As a molecule, water is an asymmetric top with the angle between H-O of  $104,45^\circ$ . As the asymmetric top water molecule is characterized by three quantum numbers which are denoted as  $J_{K_a K_c}$  and they correspond to the total internal angular momentum of a molecule and its projection onto the molecular inertial axes. The water molecule occurs in two different spin configurations: ortho- and para-water,

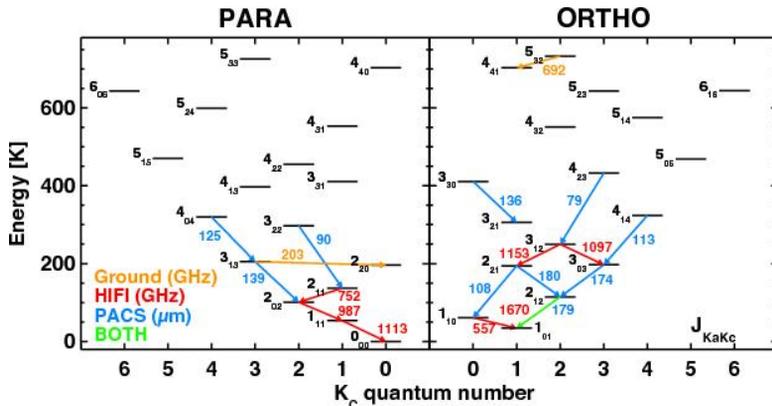


Fig. 1: Para and ortho ladders of  $\text{H}_2\text{O}$  energy rotational levels (van Dishoeck et al., 2011)

which do not interconvert due to collisions which correspond to even (para- $\text{H}_2\text{O}$ ) or odd (ortho- $\text{H}_2\text{O}$ )  $K_a + K_c$  quantum numbers. Thus it is possible to treat these spin configurations separately. The energy levels of  $\text{H}_2\text{O}$  are shown in Fig. 2.

#### 4 Calculations with MOLSCAT

The quantum inelastic scattering calculations can be solved by integrating the so-called close-coupling equations. The scattering wavefunction is represented as the product of the molecular wavefunctions and the radial part which is subsequently matched to the appropriate asymptotic form, from which we deduce the S-matrix and cross sections. Such calculations can be performed using the MOLSCAT package<sup>1</sup> (Hutson & Green, 1994). In our calculation, we use a 5D potential energy surface appropriate for rigid-rotor molecules. The potential was calculated using the coupled-cluster theory CCSD(T), which considers singles and doubles level perturbation correction for triple excitations (Faure et al., 2005). Our calculations of the  $\text{H}_2\text{O} + \text{H}_2$  collisions consider  $\text{H}_2\text{O}$  levels between  $j = 11$  and  $j = 13$  and para- $\text{H}_2$  for ground state. Fig. 2 shows the  $\text{H}_2\text{O}-\text{H}_2$  interaction potential expanded in angular functions.

#### 5 Conclusions

Since our project is in a testing phase, we have so far obtained a few cross-sections for  $J = 12$   $\text{H}_2\text{O}$  level for a range of energy (up to  $300 \text{ cm}^{-1}$ ). Once the tests are completed, we will be able to compare our results for low-energies with previous work and then expand the energy range up to  $1000 \text{ cm}^{-1}$ . Ultimately we want to expand our calculations for bigger base  $\text{H}_2\text{O}$  for  $j = 0$  to  $j = 12$  and also include ortho- $\text{H}_2$  in our calculations. We are planning to use 9-D potential taking into account vibrations between atoms and to calculate collisions at high temperatures  $T \geq 3000 \text{ K}$ . Also, we will consider calculation of potential energy surface for strongly stretched chemical bonds. This involves tests of new ab-initio methods based on symmetry-adapted

<sup>1</sup><https://www.giss.nasa.gov/tools/molscat/>

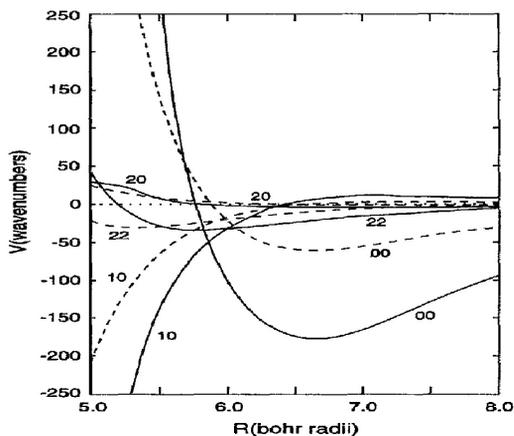


Fig. 2: H<sub>2</sub>O potential expanded in angular functions (Phillips et al., 1994)

perturbation theory extensions combined with pair coupled-cluster approach.

*Acknowledgements.* MŻ acknowledges support from the Toruń Astrophysics / Physics Summer program (TAPS 2017). AK is supported by the Polish National Science Center grants 2013/11/N/ST9/00400 and 2016/21/D/ST9/01098.

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