

He衝突によるortho-H₂Oの回転脱励起

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Introduction

Rotational excitation and quenching of molecular species collision with atoms or molecules is an important process in fields of astrophysics and atmospheric science, and had been researched by the experiments, the observations and the theoretical calculations. Helium is a lot of atoms that exist in universe after hydrogen, and one of the components of the solar wind. Water is a principal ingredient of the comet coma (temporary atmosphere formed when it approaches the sun), and one of the interstellar molecules. The meaning of this research is in the point that the finding of the rotational de-excitation in an atom and a molecular collision is able not only to be obtained but also to obtain the data of a temperature and an atmospheric density of the star.

The rotational energy levels of the H₂O molecule is labeled as $j_{k-1,k+1}$, where $k-1$ and $k+1$ are quantum number in the limit of prolate and oblate. In 2007, Yang and Stancil reported rotational quenching cross sections and state-to-state rate coefficients from initial levels $1_{1,0}$, $2_{1,2}$, and $2_{2,1}$ of ortho-H₂O and $1_{1,1}$, $2_{0,2}$, $2_{1,1}$, and $2_{2,0}$ of para-H₂O by the collision with He atom in the collision energy region from 10^{-6} to 10^3 cm⁻¹ [1]. Close-coupling (CC) and coupled state (CS) approximation scattering calculations for the rotational quenching from initial levels of $1_{1,0}$, $2_{1,2}$, $2_{2,1}$, $3_{0,3}$, $3_{1,2}$, $3_{2,1}$, $3_{3,0}$, $4_{1,4}$, $4_{2,3}$ of ortho-H₂O due to collision with He atom for collision energy between 10^{-6} to 10^4 cm⁻¹ are investigated.

Theoretical Method

Water is an asymmetric top molecule. It was thought that ortho-H₂O was handled as rigid rotor, and the conversion of ortho-H₂O and para-H₂O did not happen. The potential energy surface calculated by Patkowski *et al.* using the symmetry-adapted perturbation theory (SAPT) method [2] was used for this calculation.

When the collision energy is 10^4 cm⁻¹, the number of rotational levels of the ortho-H₂O becomes more than 300. If there are 300 rotational levels in input data, the large amount of computing time might be required. The rotational energy level of water was considered by 66 levels in total as input data for reducing the computing time. The 49 rotational levels calculated by Kyrö [3] and the 17 ones obtained by the experiment of Lanquetin *et al.* [4] were used. From the lowest rotational energy, the levels strictly were input up to 1500 cm⁻¹, and some rotational levels were chosen from 1500 to 10^4 cm⁻¹.

Close-coupling method was used to calculate rotational quenching cross sections in energy region from 10^{-6} to 450 cm⁻¹, coupled state approximation was used from 500 to 10^4 cm⁻¹. All this calculations were performed using the nonreactive scattering code MOLSCAT [5]. To calculate the state-to-state rate coefficients from 10^{-5} to 4000 K, the CC and CS calculations were included for the collision energy between 10^{-6} and 10^4 cm⁻¹. In each collision energy, enough number of the total angular momentum partial waves was included to ensure the convergence of the inelastic cross section. The maximum values of the total angular momentum quantum number J employed in the

calculations was 140. All calculations include several closed channels to ensure the convergence of the inelastic cross section.

Result

The two results calculated by using the CC and CS were compared to confirm whether the calculation of the CS approximation is effective from which energy. The results of the total cross section for the quenching from initial level $3_{0,3}$ of ortho- H_2O by collisions with He atoms were shown in FIG. 2. The results by CC and CS were corresponding well in the collision energy more than 50 cm^{-1} . From the above-mentioned, it has been understood that it was an effective method to calculate the cross section by the CS approximation in the energy region more than 450 cm^{-1} for reducing the computing time.

In the poster, state-to-state rotational quenching cross sections from an initial rotational level $3_{0,3}$ and total quenching cross section from $1_{1,0}$, $2_{1,2}$, $2_{2,1}$, $3_{0,3}$, $3_{1,2}$, $3_{2,1}$, $3_{3,0}$, $4_{1,4}$, $4_{2,3}$ are put. State-to-state quenching rate coefficients were compared with the result reported by Green in 1993.

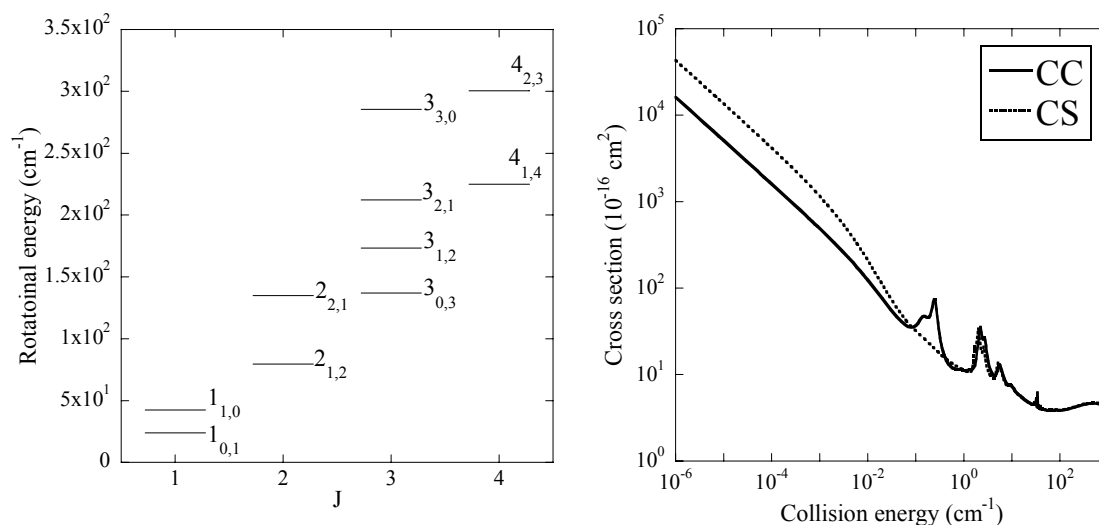


FIG.1 (Left figure) Rotational levels of ortho- H_2O for initial state in present calculations.

FIG.2 (Right figure) Total cross section for quenching of ortho- H_2O (initial level $3_{0,3}$) by collisions with He atoms as functions of collision energy.

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