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 H$_2$O 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-H$_2$O and $1_{1,1}$, $2_{0,2}$, $2_{1,1}$, and $2_{2,0}$ of para-H$_2$O 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-H$_2$O due 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-H$_2$O was handled as rigid rotor, and the conversion of ortho-H$_2$O and para-H$_2$O 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-H$_2$O 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 $10^{5}$ 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$_2$O 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 $1_{1,0}$, $2_{1,2}$, $2_{2,3}$, $3_{0,3}$, $3_{1,2}$, $3_{2,1}$, $3_{3,0}$, $4_{1,4}$, $4_{2,3}$ are put. State-to-state quenching rate coefficients were compared with the result reported by Green in 1993.

**References:**


