Study of the bending relaxation of water by collision with Ar.

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Water is one of the most abundant molecules in the universe. It is the most abundant polyatomic molecule in our galaxy and the third most abundant molecule in the interstellar medium after H_2 and CO, where it plays an important role in the chemistry of interstellar clouds. Transitions involving some of its rovibrationally excited levels have recently been detected and it becomes essential to know its collision rates with the most abundant elements in the interstellar medium (H_2, He, H, and e-). Such studies exist for the fundamental vibrational level and considering water as a rigid rotor [1, 2]. The methodology necessary to deal with the vibrationally excited levels which takes into account the coupling between bending and rotation of the water molecule has recently been developed [3, 4]. It must now be tested against experiment and experimental data are already available for collisions with argon. This is the reason why this system was chosen, as new experiments involving vibrationally excited levels are also underway in the laboratory. In order to be able to perform the dynamics calculations, a new 4D potential energy surface including the water bending has been developed and describes rigorously the long and short range behaviors. Inelastic dynamics calculations are performed and compared to experimental data as well as to the results of previous theoretical studies. These results will be presented and analyzed.

Index Terms: bending relaxation, inelastic collisions,close coupling method, potential energy surface

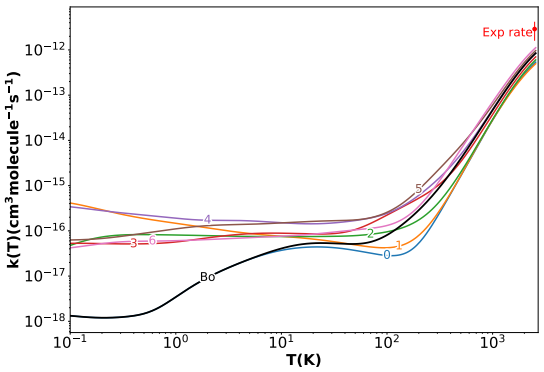

Figure 1: Comparison with the experiments [5] of the j state selected and Boltzmann averaged vibrational quenching rate coefficients of the j=0,1,2,3,4,5,6 rotational states belonging to the first excited bending level of water induced by the collision with Ar.

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