CHAPTER I

INTRODUCTION

Ordinary water is a mixture of several species differing in molecular weight. There are at present three known isotopes of hydrogen (^{1}H, ^{2}H, ^{3}H), and six of oxygen (^{14}O, ^{15}O, ^{16}O, ^{17}O, ^{18}O, ^{19}O). The relative abundances of $H_2{}^{18}O$, $H_2{}^{17}O$, and HDO in the natural water are 0.2 per cent, 0.04 per cent, and 0.03 per cent respectively.

Although water is very common, many properties of water are regarded as strange. Ice floats in water which means that the density of liquid water is higher than that of ice. Other liquids are less dense than when being solid. Water has unusually high heat capacity compared to other liquids. Together with other anomalous properties such as high dielectric constants, it exhibits minimum compressibility etc. There is no theory to explain all properties accurately.

At present two major models of liquid water can account for certain properties of water; they are the mixture model and the distorted hydrogen bond model[1].

The mixture model postulates that there are several species of clusters of water molecules in liquid water. The interstitial models are a class of mixture models in which one of the species forms a hydrogen-bonded framework, and the other species resides in cavities that exists in this framework. Thus it explains the higher density of liquid water than that of ice.

As temperature gets higher more bonds of ice cluster are broken. The energy in breaking the bonds amounts to the high heat capacity of water.

In the distorted hydrogen bond models, hydrogen bonds are regarded as distorted to varying degrees, rather than as either intact or broken as in mixture models. Water molecules in the liquid, like those in the ices, are considered to be four-coordinated; but the networks of linked molecules in the liquid are irregular and varied. It is believed that five-membered rings are a frequent configuration in the liquid, but rings containing four, six, seven, or even more molecules are also present. This model could also explain the density and heat capacity of water .

To understand better on properties of water a more rigorous and accurate theory of the liquid water is needed. Investigation on properties of liquid water is still in common interest.

Proton nuclear spin relaxation in water has been studied very extensively since the first theory and measuring methods were developed by Bloembergen, Purcell and Pound[2] in 1948, and later modified by Kubo and Tomita[3] in 1954. Both of these papers showed that the spin-lattice relaxation of a single nuclear spin in a liquid is induced by the fluctuating local magnetic field of the neighboring spins. The spin-lattice relaxation time (T_1) is the characteristic time in which magnetization of nuclear spins reaches their equilibrium in the magnetic field direction. The spin-lattice relaxation involves transfering of energy from

the spin system to the structure or lattice. In the theory rotational and translational motions are proposed to induce the nuclear relaxation.

Simpson and Carr[4] measured the diffusion coefficient and the spin-lattice relaxation time of protons in ordinary water and concluded that the Stokes-Einstein relation adequately describes the relative temperature dependence of viscosity and diffusion, but that above temperature about 40°C the spin-lattice relaxation does not follow the viscosity in the predicted manner.

The purpose of this investigation was to measure the temperature dependence of the spin-lattice relaxation time, T_1, and the transverse relaxation time, T_2, in pure water by pulse nuclear magnetic resonance in order to gain understanding of liquid water.