RADIATIVE LIFETIME FOR NUCLEAR SPIN CONVERSION OF WATER-ION, H_2O^+

KEIICHI TANAKA, *Department of Applied Chemistry, National Chiao Tung University, Hsinchu, 30010, TAIWAN and Department of Chemistry, Faculty of Sciences, Kyushu University, Fukuoka, 812-8581 JAPAN*; KENSUKE HARADA, *Department of Chemistry, Faculty of Sciences, Kyushu University, Fukuoka, 812-8581 JAPAN*; TAKESHI OKA, *Department of Astronomy and Astrophysics and Department of Chemistry, the Enrico Fermi Institute, the University of Chicago, Chicago, Illinois, 60637, USA.*

Nuclear spin conversion interaction of the water ion, H_2O^+, has been studied to derive the spontaneous emission lifetime between the *ortho*- and *para*-levels. The H_2O^+ ion is a radical with $^2B_1$ electronic ground state and the off-diagonal electron spin-nuclear spin interaction term, $T_{ab}(S_a\Delta I_b + S_b\Delta I_a)$, connects *para* and *ortho* levels, because $\Delta \boldsymbol{I} = \boldsymbol{I}_1 - \boldsymbol{I}_2$ has nonvanishing matrix elements between $I = 0$ and 1. The T_{ab} coupling constant, derived by an $ab\ initio$ calculation in MRD-CI/Bk level to be 72 MHz, is larger than that of H_2O by 4 orders of magnitude, makes the $ortho$ to $para$ conversion of H_2O^+ faster than that of H_2O by 8 orders of magnitude and possibly competitive with other astrophysical processes.

Last year we reported *ortho* and *para* coupling channels below 900 cm^{-1} caused by accidental near degeneracy of rotational levels.[a] For example, hyperfine components of the $4_{2,2}(o)$ and $3_{3,0}(p)$ levels mix each other by 1.2 x 10^{-3} due to the near degeneracy (ΔE = 0.417 cm^{-1}), but the lower lying $1_{0,1}(p)$ and $1_{1,1}(o)$ levels mix only by 8.9 x 10^{-5} because of their large separation (ΔE = 16.27 cm^{-1}). In the present study, we solved the radiative rate equations including all the rotational levels below 900 cm^{-1} to give the *o-p* conversion lifetime to be 0.451, 3.27, 398 and 910 years for the equilibrium o/p ratio of 3.00, 3.00, 4.52, and 406 when the radiation temperature T_r is 100, 60, 20 and 5 K.

These results qualitatively help to understand the observed high o/p ratio of 4.8 $\pm$ 0.5 (corresponding to the nuclear spin temperature of 21 K) toward Sgr B2,[b] but they are too slow to compete with the reaction by collision unless the number of density of H_2 in the region is very low ($n \sim$1 cm^{-3}) or the radiative temperature is very high ($T_r >$ 50K).[c]

[a] K. Tanaka, K. Harada, and T. Oka, *the 67th OSU Symposium* MG06, 2012.

[b] P. Schilke, et al., *A&A* **521**, L11 (2010).

[c] K. Tanaka, K. Harada, and T. Oka, *J. Phys. Chem. A*, $in\ press$.