SPONTANEOUS EMISSION BETWEEN ORTHO- AND PARA-LEVELS OF WATER-ION, H_2O^+

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Nuclear spin conversion interaction of water ion, H_2O^+, has been studied to derive spontaneous emission lifetime between *ortho*- and *para*-levels. H_2O^+ is a radical ion with the $^2B_1$ electronic ground state. Its 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 mixing by this term with T_{ab} = 72 MHz predicted by $ab\ initio$ theory in the MRD-CI/Bk level,[a] is many orders of magnitude larger than for closed shell molecules because of the large magnetic interaction due to the un-paired electron. Using the molecular constants reported by Mürtz et al. by FIR-LMR[b], we searched for *ortho* and *para* coupling channels below 1000 cm^{-1} with accidental near degeneracy between *para* and *ortho* levels. For example, hyperfine components of the $4_{2,2}(ortho)$ and $3_{3,0}(para)$ levels mix by 1.2 $\times$ 10^{-3} due to their near degeneracy (ΔE = 0.417 cm^{-1}), and give the *ortho-para* spontaneous emission lifetime of about 0.63 year. The most significant low lying $1_{0,1}(para)$ and $1_{1,1}(ortho)$ levels, on the contrary, mix only by 8.7 $\times$ 10^{-5} because of their large separation (ΔE = 16.267 cm^{-1}) and give the spontaneous emission lifetime from $1_{0,1}(para)$ to $0_{0,0}(ortho)$ of about 100 year.These results qualitatively help to understand the observed high *ortho*- to *para*- H_2O^+ ratio of 4.8 $\pm$ 0.5[c] toward Sgr B2 but they are too slow to compete with the conversion by collision unless the number density of the region is very low ($n \sim$ 1 cm^{-3}) or radiative temperature is very high ($T_r >$ 100 K).

[a]M. Staikova, B. Engels, M. Perić, and S.D. Peyerimhoff, *Mol. Phys.* **80**, 1485 (1993)
[b]P. Mürtz, L.R. Zink, K.M. Evenson, and J.M. Brown *J. Chem. Phys.* **109**, 9744 (1998).
[c]LP. Schilke, et al., *A&A* **521**, L11 (2010).