Conversion of nuclear spin isomers of methanol in the gas phase

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Nuclear spin isomers (NSIs) are modified molecules by differing states of nuclear spins[1]. The methanol (CH_3OH) molecule has the torsion of the CH_3 group and of the OH group with respect to each other[2]. From the three spin–1/2 hydrogen nuclei of this CH_3 group, the ortho and para NSIs of methanol are formed. The former has a total nuclear spin quantum number I = 3/2, and the latter is of I = 1/2. Conversion of NSIs of gaseous methanol from a non-equilibrium concentration of them created by the pumping of a CO_2 gas laser can be induced by non-magnetic molecular collisions. We show in this study that the perturbation potential caused by the weak hyperfine interactions of nuclear spin-spin (SS) and nuclear spin-rotation (SR) in CH_3OH can mix the near-degenerate ortho-para states of methanol, which are doorway channels in the interconversion of ortho-para methanol. A theoretical model of such an interconversions in CH_3OH has been developed, the mixed pairs of the quantum ortho-para states of the CH_3OH with the energy intervals less than 50 MHz have been calculated[2], and numerical calculations of the CH_3OH conversion rates due to the interactions of SS and SR have been carried out. The total conversion rate at room temperature and at a pressure of 0.8 Torr in CH_3OH was found to be about 10^{-2} s^{-1}. This is the largest conversion rate between two NSIs during the quantum relaxations[3] among the gases of CH_3OH, CH_3F, and C_2H_4.

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References

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