FORBIDDEN ROTATIONAL TRANSITIONS AND ASTROPHYSICS

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When I read Townes and Schawlow's textbook as a beginning student, I was puzzled by the symmetric top selection rule ΔK = 0, because this rule corresponds to cylindrical symmetry C_∞; applying it to NH_3 with C_3 symmetry cannot be right. At that time, however, I did not pursue how this wrong rule affect the actual spectrum. 10 years later interstellar NH_3 was discovered by Townes' group. When I read the discoverers' claim that lifetimes of (J, K) = (2,2) and (3,3) metastable levels are "longer than the lifetime of the Universe", it was obvious that this wrong statement resulted from the wrong ΔK = 0 selection rule. Accurate theory[a] gave the life times of the (2,2) and (3,3) metastable levels to be 230 years and 44 years, respectively, 10^8 times shorter than the lifetime of the Universe. The theory also predicted $\Delta k = \pm 3$ pure rotational transitions which were observed for PH_3, PD_3 and AsH_3[b]

In this paper[c] I calculate spontaneous emission via forbidden transitions for astrophysically important symmetric tops; oblate tops NH_3, H_3O^+, H_3^+, and prolate tops CH_3CN. These calculations are preparations for future analyses of ther thermalization.

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[a] T. Oka, F.O. Shimiza, T. Shimizu, J.K.G. Watson, ApJ 165, L15 (1971)

[b] F.Y. Chu, T. Oka, J. Chem. Phys. 60, 4612 (1974)

[c] T. Oka, J. Mol. Spectrosc. 379, 111482 (2021)