

CH₃ INTERNAL ROTATION IN 9-METHYLANTHRACENE

MASAAKI BABA, *Division of Chemistry, Graduate School of Science, Kyoto University, Kyoto, Japan*;
MASATOSHI MISONO, *Applied Physics, Fukuoka University, Fukuoka, Japan*; JON T. HOUGEN, *Sensor Science Division, National Institute of Standards and Technology, Gaithersburg, MD, USA*.

We observed the rotationally resolved fluorescence excitation spectrum of the $S_1 \leftarrow S_0$ transition of jet-cooled 9-methylantracene. The potential energy curve for CH₃ internal rotation is six-fold symmetric. The barrier to rotation (V_6) is $\sim 120 \text{ cm}^{-1}$ [2], which is considerably larger than that of toluene ($\sim 5 \text{ cm}^{-1}$) [1]. The V_6 value is the energy difference between two isomers 'staggered' and 'eclipsed'. The main contribution to V_6 is expected to be hyperconjugation, which is the π -like interaction between the aromatic π orbital and methyl sp^3 orbital.

The final goal of this work is to quantitatively elucidate the vibrational and rotational energy levels for CH₃ internal rotation. It is essential to observe the high-resolution and high-precision electronic spectra and theoretically search the best effective Hamiltonian to reproduce the experimental results. We are now developing a new laser control system with optical frequency comb locked to GPS, and an ab initio method which provides the reliable potential energy curve.

[1] M. Baba, et al., *J. Phys. Chem. A* **113**, 2369 (2009)

[2] D. R. Borst and D. W. Pratt, *J. Chem. Phys.* **113**, 3658 (2000)