METHYL TORSIONAL LEVELS IN 9-METHYLANTHRACENE

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We have analysed energy levels of CH_3 torsion in the S_0 and S_1 states of 9-methylanthracene (9MA) by high-resolution fluorescence excitation spectrum in a supersonic jet. 9MA has the G_{12} molecular symmetry, which is the same as toluene. The sixfold torsional barrier in toluene is very small, [a] and the barrier height has been accurately determined as $V_6(S_0)$ = 4.874 cm^{-1} and $V_6(S_1)$ = 26.376 cm^{-1} by microwave and ultrahigh-resolution laser spectroscopy. [b,c] In 9MA, we estimated the barrier height as $V_6(S_0) \approx 100$ cm^{-1} and $V_6(S_1) \approx 50$ cm^{-1}, which is remarkably larger than that in toluene. The difference of transition energies between the $0a_1' \rightarrow 0a_1'$ and $1e'' \rightarrow 1e''$ is expected to be about 1 cm^{-1}. We have observed rotationally resolved ultrahigh-resolution spectrum of 9MA in a collimated molecular beam and confirmed this splitting. All of the observed rotational lines exhibit B-type selection rule, and the direction of transition moment has been shown to be parallel to the C_3 axis of the CH_3 group.

[a] P. J. Breen, J. A. Warren, E. R. Bernstein, and J. I. Seeman, *J. Chem. Phys.*, **87**, 1917 (1987)
[b] W. A. Kreiner, H. D. Rudolph, and B. T. Tan, *J. Mol. Spectrosc.*, **48**, 86 (1973)
[c] D. R. Borst and D. W. Pratt, *J. Chem. Phys.*, **113**, 3658 (2000)