Internal Reorientational Dynamics of Methyl Group in 2,6-Dichlorotoluene

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^{13}C relaxation measurement for methyl group in 2,6-dichlorotoluene may be utilized as a criterion for evaluation of the reorientation dynamics of internal rotor. To see how the symmetric internal rotor works rotational diffusion model and extended diffusion model have been numerically tested together with diffusion in a potential which encompasses the intermediate character of diffusion and jump among the nearest potential wells. With the aim of clearly elucidating the reorientation of the methyl rotor we have analytically solved the general jump model with three different rate constants in a 6-fold potential barrier and applied to the present internal rotor. Assuming that internal rotation of methyl group in 2,6-dichlorotoluene can be described in terms of jumps among six-fold harmonic potential wells, we could conclude the rate for 6-fold jump is at least 1.53 times as great as that for 3-fold jump. In this paper we report that the two correlation times previously obtained in our coupled