Analysis of the effect of the translational-rotational coupling on the pseudo-diffusion along the molecular axes of glass forming liquid meta-cresol: A molecular dynamics analysis

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We investigated by molecular dynamics simulations the dynamical properties (translation and rotation) of the glass-forming liquid meta-cresol. This system was investigated at 19 temperatures from T=600K down to 220K. This temperature range encompasses the liquid and glassy state of meta-cresol. In order to get insight into the coupling between the translation and rotation motions, the center of velocity autocorrelation function was calculated along the meta-cresol principal axes. We showed then that the time behavior of the velocity and angular velocity is connected to the change in the locale structure. Indeed, the long time negative region in the velocity autocorrelations was associated with a caging effect while the occurrence of a short time negative region in these functions was considered as a signature of specific interaction. The time evolution of the rotation translation coupling was evaluated from the difference $\Delta_i^{RTC}(t)$ between the velocity autocorrelation function calculated with respect to the molecular frame *(i=x,y,z)* of the meta-cresol molecule and that of the same function calculated in the frame of the hypothesis that there is no statistical correlation between the translation and rotation motions. The positive regions of $\Delta_i^{RTC}(t)$ *(i=x,y,z)* indicate an occurrence of a cooperative effect which means that the each of the two motions is realized in the favor of the other. Conversely, negative regions indicate that the rotation and translation motions are anti cooperative. The change in the local structure was investigated by using the nearest neighbor approach. The change in the radial and the mutual orientation nearest neighbor distributions is shown to be consistent with the fact that the translation rotation coupling is more effective along the x and z axes.