

Dynamics of aromatic molecules entrapped in the clathrate phase of syndiotactic polystyrene

Fumitoshi Kaneko(A), Tatsuya Kawaguchi(A), Koichi Ute(B)

Graduate School of Science, Osaka Univ.(A), Graduate School of Engineering Science, Osaka Univ.(B)

Syndiotactic polystyrene (sPS) is a relatively new commodity polymer. It exhibits a variety of crystalline states depending on crystallization conditions, alpha and beta of TT conformation and gamma, delta and empty-delta of TTGG conformation. The appearance of the delta form is one of the important characteristics of sPS. It is a clathrate crystalline phase with small molecules, such as chloroform, benzene, toluene, xylene and so forth. The guest molecules are included in the cavities between polymer sheets of TTGG helical conformation. In this study we have investigated the dynamical properties of two kinds of stored aromatic compounds, benzene and p-xylene.

In order to reduce the contribution of sPS matrix to quasielastic neutron spectra (QNS), hydrogenated guest molecule were incorporated into the cavities of sPS matrices prepared from fully deuterated styrene. All QNS spectra were measured with AGNES spectrometer of JRR3M (Tokai).

Figure 1 shows QNS spectra of the two sPS clathrates. As for the sPS(benzene) clathrate, the Q dependence of EISF suggests the rotational diffusion of benzene by jump motions among six sites around a circle with a radius of about 2.5Å, i.e., the jump motion around the six-fold rotation axis. p-Xylene shows a significant Q dependence of EISF together with a widely spread QNS components in the whole temperature region between 300 and 40 K. The Q dependence of p-xylene is much larger than that of benzene even at 100K, which cannot be attributed only to the rotational diffusion of methyl hydrogen atom by the three-site jump motion, although the methyl hydrogen atoms are the major scattering source in p-xylene. These character-

istics of the QNS spectra indicates the existence of fast and large motion of p-xylene molecules as a whole, probably a large librational motion of p-xylene.

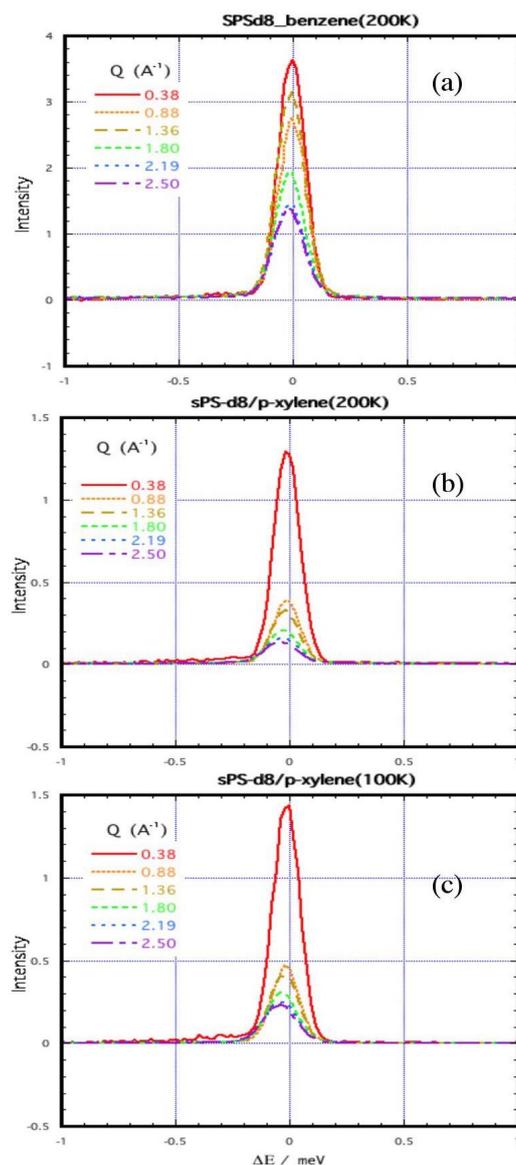


Fig. 1. QNS spectra of syndiotactic polystyrene clathrate phase containing benzene at 200K (a) p-xylene at 200K and 100K (b) and (c).