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SELF DIFFUSION OF PHTHALIC ACID ESTER MOLECULES*

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A study was made of self diffusion of molecules of several pure phthalates (dimethylphthalate, dibutylphthalate and dioctylphthalate) and their molecules added to PVC by a NMR pulse method. It was shown that the temperature relation of the coefficient of self diffusion of pure phthalates is satisfactorily described by the Einstein-Hill theory. Self diffusion of phthalates introduced in PVC is treated on the basis of the activation theory. Energies of cavity formation in diffusion of single phthalate molecules in a PVC matrix were calculated. The relation between the activation energy of self diffusion and plasticizer concentration was described. It was shown that the type of self diffusion of phthalates depends on the state of the polymer matrix.

MANY properties of plasticized polymers are determined by the type of molecular motion, particularly the mobility of plasticizer molecules, among which phthalates are often used. Thus, the brittle point of the polymer [1], the effectiveness and extraction properties of the plasticizer [2] are related to the translational mobility of molecules of the latter.

However, characteristics of the forward motion of plasticizer molecules, phthalates in particular, have been little studied. Results concerning the self diffusion of pure phthalates are generally unavailable.

When studying translational motion in a system consisting of a polymer and a low molecular weight substance classical methods are normally used, in which the coefficient of mutual diffusion, a parameter reflecting the translational mobility (self diffusion) of macro- and small molecules and the mass flows of these components [3], is measured. Coefficients of self diffusion D, which characterize the individual mobility of molecules, are obtained as a result of conversion using the theory of polymer solutions. Direct measurements of D of polymer and plasticizer molecules may be effected by NMR [4].

An attempt is made in this study to examine self-diffusion of molecules of several pure phthalates and their molecules added to PVC by a NMR pulse method.

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