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## **Influence of Transport Site Structure on Charge Carrier Mobility in Polymer Systems**

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For the doped polystyrene transport films, it was experimentally found that drift mobility decreased when disordered dipole transport molecules were oriented along the external electric field. The trend of decreasing mobility when dipole moment of molecules increases appears to be observed among derivatives of compounds of a kind.

**Keywords** hole transport, dipole molecules, doped polymer

The mechanism of charge transport in disordered media has been the subject of many studies. Molecularly doped polymers and low-weight organic compounds represent such media. They are of interest not only because of their commercial utility but also due to of the scientific appeal of amorphous hopping systems <sup>(1,2)</sup>. A strong donor or acceptor molecule provides a hole or electron transport, respectively. Drift mobilities of charge are strongly dependent on field and temperature, as well as on structure of the donor or acceptor molecule and polymer host. The charge transporting molecule (CTM) with a donor or acceptor group evidently has a dipole moment. The effect of dipole CTMs or additives on the mobility of holes was experimentally investigated in a series of studies <sup>(3-7)</sup>. Nevertheless, there is

no complete knowledge of the subject. To understand better the role of dipole CTMs and their orientation, we studied an influence of magnitude of CTM dipole moment and alignment of CTM dipoles on the drift mobility of holes in some novel transporting molecular systems and in the oriented CTM doped polymer films.

Charge transport layers under study were bisphenol-A-polycarbonate (PC) doped with phenyltolyl-naphthylamine (PTNA), binderless PTNA, polystyrene (PS) doped with triphenylamine (TPA) or 4-diethylamino-benzaldehyde-diphenylhydrazone (DEH). PTNA and DEH were supplied by K.K.Kochelev and their syntheses were described earlier<sup>(8)</sup>. TPA was from Merck. PS from BDH was supplied by Z.He. PC was from Aldrich. All the CTMs provide the hole transport.

The charge carrier transport was studied by standard time-of-flight (TOF) techniques<sup>(1)</sup>. Sandwich type samples were prepared for the measurements. Films were produced by dissolving a mixture of polymer and TPA (30 wt.%), DEH (30 wt.%) or PTNA (50 wt.%) in the corresponding solvent. Then the solutions were cast onto quartz substrates with ITO electrode followed by drying at room temperature for 24 hours or more. The binderless PTNA samples were prepared by vacuum thermal sublimation from a resistance-heated quartz crucible onto a substrate. The crucible temperature was in the range 220-240°C and adjusted such that the deposition time ranged between 2-3 minutes. The temperature of substrate increased during the evaporation time from the room temperature up to 60°C. Finally, a 0.3  $\mu\text{m}$  generation layer of Se and an aluminum semitransparent electrode were vapor deposited on the top free surface of each sample in vacuum of  $10^{-6}$ - $10^{-5}$  Torr. Thicknesses of the layers under study were 3 and 15  $\mu\text{m}$ .

In order to provide the orientation of the CTM dipoles perpendicularly to the film surface, the doped PS film coated onto the electroconductive

substrate was heated for 90-120 s in the thermostatic chamber at 71-76 °C (near PS glass transition temperature,  $T_g = 81$  °C) and then an uniform electrostatic charge was deposited on a part of the film surface for 15-40 s at the same temperature. The charging was performed by a corona discharge arising between grounded ITO electrode and a pin which served as a negative electrode. Finally, to fix the dipole orientation the samples were cooled to room temperature under the corona discharge for about 2 min. For TOF measurements, a generation layer and an opposite electrode were deposited on the film surface as written above.

The measurements were carried out in a small current mode of the TOF experiment. The transient currents were measured by a digital oscilloscope Tektronix TDS340A. The transit times,  $t_T$ , were determined from the intersection of asymptotes to the plateau and trailing edge of the transients. The drift mobilities were determined from the conventional expression  $\mu = d/(F t_T)$ , where  $F$  is the applied electric field,  $d$  is the film thickness.

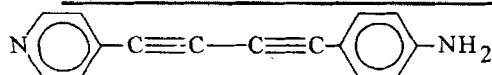
In Table 1, the data represent hole mobility in the limit of zero-field strength and dipole moment for two different types of CTM: triarylamine and diacetylene (DA) derivatives. The molar concentration of tritolylamine (TTA) and PTNA are close in magnitude. Dipole moment for the CTMs with the exception of TTA were calculated by the PM3 method. For the DA compounds (Fig.1.), mobility was studied in the earlier work <sup>(9)</sup>. As is seen, the mobility in the PC+PTNA system with larger dipole moment of the CTM is considerably lower than that in PC+TTA. Similar correlation of mobility and dipole moment exists in a series of the binderless DAs. However, the correlation is not the case when binderless PTNA and DAs are compared, so such a correlation appears to exist among derivatives of CTM of a kind. Therefore, a theory for mobility dependence on dipole nature of CTMs seems

to be more complicated and a mutual orientation of CTMs must be allowed for.

Influence of dipole CTM alignment on mobility was studied in PS films doped with TPA (0.87D) or DEH (3.32D) molecules. The effect of the corona poling on dipoles in the film manifested itself in the decrease of absorption (spectra are not shown) which was unambiguously associated with an orientation of CTM along the corona field direction. For the PS+TPA system, the field dependence of the hole drift mobility for both pristine and corona poled films is shown in Fig.2. The similar dependence was observed in the PS+DEH films. When dipole vectors were previously oriented in the direction parallel with the electric field in the TOF measurement, the decrease of the mobility may be explained in the following manner. The positive charge is predominantly localized on the *N* atom (for DEH, on the *N* atom of the hydrazone). Thus, an electron needs to overcome some extra steric and electrostatic barriers caused by rest of molecule moieties to be transferred between the neutral and cation radical molecules. In the disordered system, where dipoles are not aligned along field strongly, the favorable mutual orientation of molecules exists at which the extra barrier is negligible.

TABLE 1. Hole transport compositions and their parameters.

Composition	CTM concentration, wt. %	Dipole moment of CTM, Debye	$\mu (F=0)$ , $\text{cm}^2/(\text{V s})$	Ref.
PC+TTA	45	0.9	$2.5 \cdot 10^{-5}$	1
PC+PTNA	50	1.28	$1.0 \cdot 10^{-7}$	
PTNA	100	1.28	$0.8 \cdot 10^{-6}$	
DA-1	100	3.77	$2.1 \cdot 10^{-6}$	9
DA-2	100	3.90	$2.2 \cdot 10^{-6}$	9
DA-3	100	2.61	$2.4 \cdot 10^{-5}$	9



DA-1

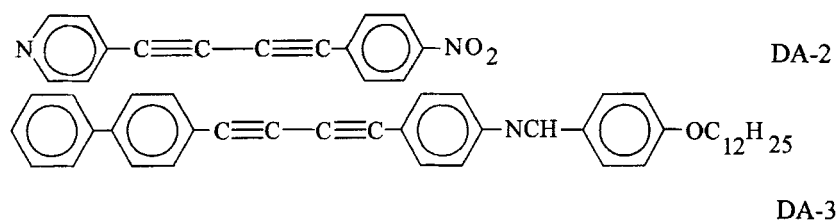


FIGURE 1. Molecular structures of the diacetylene compounds

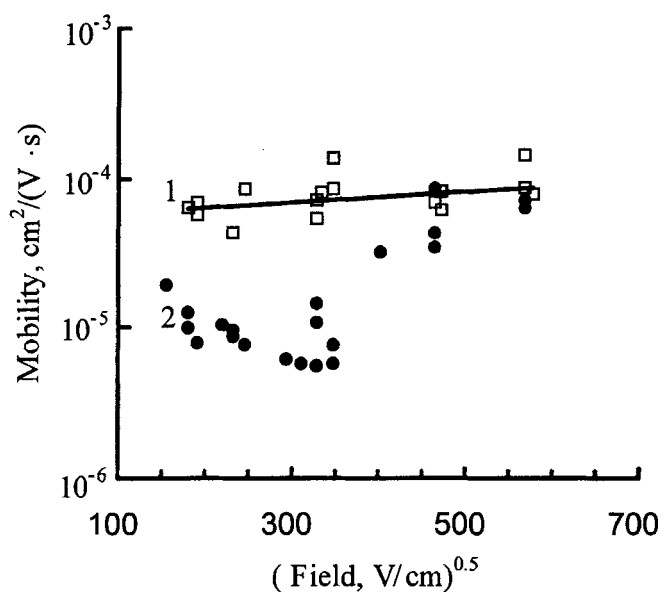


FIGURE 2. Field dependence of the hole drift mobility in the pristine (1) and treated (2) PS+TPA films.

There is a simple model of randomly oriented dipoles of the transport sites which agrees well with the most characteristic features of the charge carrier transport in disordered organic media<sup>(10)</sup>. The model can be used to explain the obtained data. The following general conclusions may be drawn on the base of Monte Carlo simulation of the electrostatic potential distribution over the whole sites and the charge transport

process. At moving from the disordered orientation system to the ordered one absolute values of the mobility are decreased.

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