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Drift Mobilities of Electrons and Holes in Single Crystals of Anthracene-1,3,5-Trinitrobenzene Charge-Transfer Complex

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Drift Mobilities of Electrons and Holes in Single Crystals of Anthracene—1,3,5-Trinitrobenzene Charge-Transfer Complex

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In view of the basic difficulties encountered in growing pure crystals of organic molecular complexes the anthracene-1,3,5-trinitrobenzene (AN–TNB) is taken as a model substance for studying electrical and photoelectrical properties of weak charge-transfer complexes. The monoclinic unit cell of the 1 : 1 AN–TNB system[1] comprises four molecules of the complex, the component molecules being stacked alternatively plane to plan forming infinite columns extended along the *c*-axis. The planes of the aromatic rings of the anthracene and trinitrobenzene molecules make an angle of 83° with the *c*-axis. The closest intermolecular contacts are formed by adjacent molecules.

Both the conductivity and mobility measurements[2] reveal the existence of a phase transformation in AN–TNB system at about 350 K, the structure of the high temperature phase being unknown. The results presented in this communication concern the variation of the charge carrier mobilities with temperature and crystallographic direction for the low temperature phase of an AN–TNB crystal.

Single-crystalline boules of AN–TNB were grown in a sublimation furnace by a method similar to that described by Radomska *et al.*[3] The zone-refined materials: anthracene and 1,3,5-trinitrobenzene were melted together in stoichiometric amounts and then zone-melted again in order to obtain the exact molal ratio.[4] The single crystalline ingots grown from the vapour phase were large enough to cut several differently oriented crystal plates from a boule. The drift mobilities of carriers of either sign were determined by "transit time"[5,6] measurements. The dashed lines in Figure 1 and Figure 2

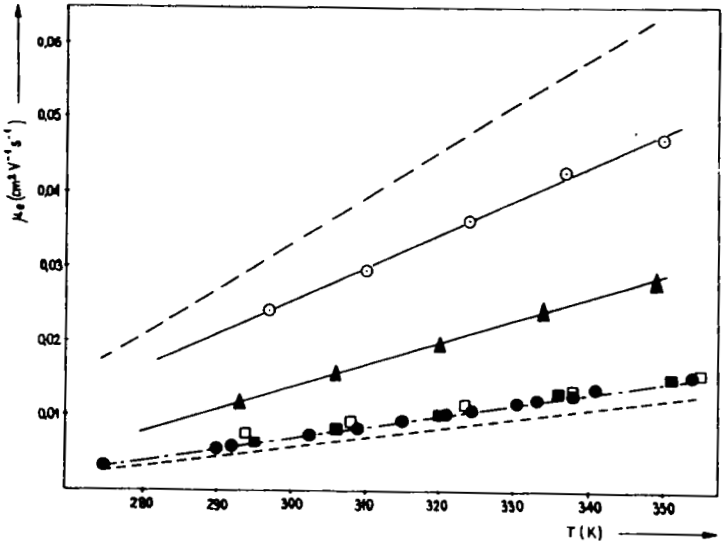

FIGURE 1

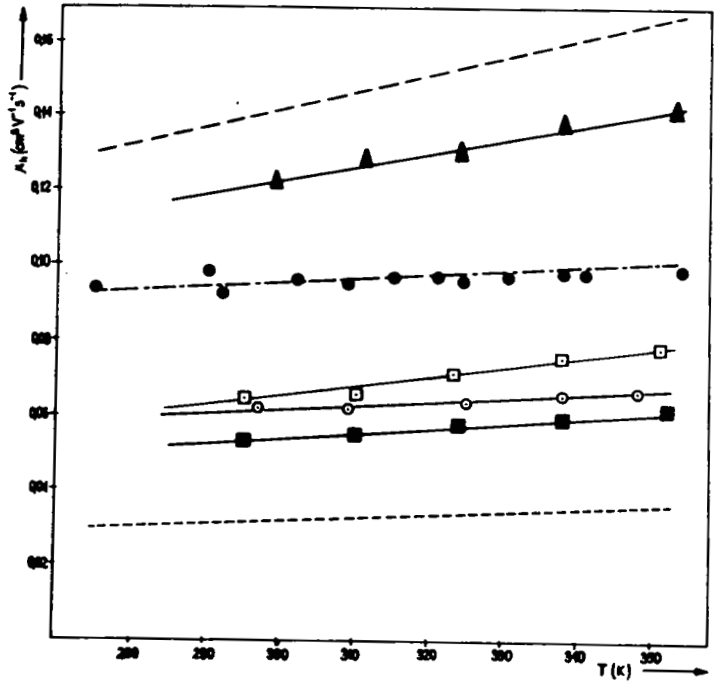

FIGURE 2

Electron (Figure 1) and hole (Figure 2) mobilities in the low temperature phase of AN–TNB charge-transfer complex measured on five differently oriented crystals. The full circles refer to the mobilities measured in the direction of the twofold axis b. The dashed lines (averaged values) refer to the principal components of the mobility tensor: μ_1 (lowest mobilities), μ_2, μ_3 (highest mobilities).

refer to the principal components of the mobility tensor calculated by averaging[7] the experimental data for five differently oriented crystals.

According to the Von Neumann principle, the orientation of the tensor axes x_1, x_2, x_3 in relation to the orthogonal system a^*, b, c (a^* being perpendicular to the crystallographic axes b, c of the monoclinic system) is constrained so that the x_2-axis coincides with the twofold b-axis. In AN–TNB system the axes of the electron mobility tensor coincide (within the experimental error) with the a^*, b, c axes. The direction of "good conduction" for electrons is parallel to the c-axis (confirming the presumption that the most probable process for the motion of an excess electron is that of jumping between acceptor and donor molecules stacked along the c-axis), electron mobility in the a^*b plane (corresponding approximately to the plane of aromatic rings) being explicitly lower and practically isotropic. The mobility of holes is surprisingly high and shows very weak temperature dependence. The most probable path of hole transport deviates from that of electrons; the angle (taken from a^* to c) which makes the system of the axes x_1, x_3 of the hole mobility tensor in relation to the a^*, c axes system was found to be about 33°. It is possible that the migration of holes should be governed by a mechanism different from the mechanism of electron transfer.

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