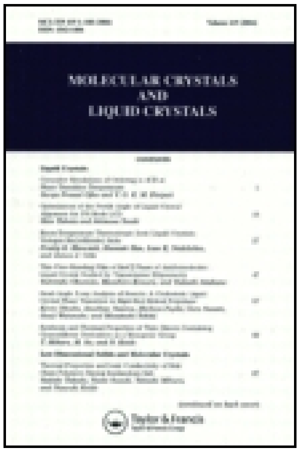

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Temperature Dependence of Current Carriers Mobilities in Anthracene

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Temperature Dependence of Current Carriers Mobilities in Anthracene

(Comment)

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In a recent paper,[1] hereafter referred to as (1) Chojnacki has reported calculation of transfer integrals in anthracene crystal at both room and low temperature (290 °K, 95 °K). He uses Slater atomic wave functions with an exponent $\alpha = 3.08$ Å^{-1}, together with Hückel coefficients, in order to build the molecular wave function of the excess electron (or hole) on an anthracene molecule. The crystal structure at those two temperatures was studied by Mason[2] who showed that there was not only a change in the dimensions and the angle of the monoclinic unit cell but also slight rotation of the molecules within this unit cell.

The T.I. values (squared) enter in the expression of mobility. Therefore the temperature dependence of the mobility can be explained by an evential variation of the transfer integrals with temperature due to a temperature induced change of the relative equilibrium positions of the different molecules. However due to the Einstein relation between mobility and the diffusion constant there is already a T^{-1} dependence of the mobility with temperature. A departure of the experimental values from this T^{-1} dependence may be explained for instance by a T.I. variation with temperature, but also by a temperature dependence of the scattering factor, or even (according to Gosar and Choi[3]) by the influence of a phonon assisted part of the mobility which is obviously dependent upon the density of phonons, which in turn is linearly proportional to T.

Our comment will be limited to the discussion of Chojnacki's result, and not devoted to a general study of the temperature dependence of the carriers mobility in anthracene.[4] We have summarized in Table 1 all the T.I. values computed with the same assumptions as Chojnacki used. One difference between those results is related to the number of carbon atoms which are included in the calculation, whether one selects atoms at distances smaller than 5 Å, 10 Å or one considers all the carbon atoms belonging to the two involved molecules. Another difference is due to a slight reported difference in the anthracene room temperature crystallographic structure when measured by Cruickshank[5] and by Mason.[2]

TABLE 1 Transfer integrals values between central molecule and molecule (010), (1/2 1/2 0) (1/2 1/2 1). All units are in 10^{-4} eV.

Authors		Molecules					
		010		1/2 1/2 0		1/2 1/2 1	
		+	−	+	−	+	−
Chojnacki[1]							
	290 °K	− 23.20	17.60	− 17.43	− 25.00	− 1.69	− 0.58
	95 °K	− 3.81	17.57	+ 8.25	− 32.74	− 7.52	+ 0.78
Leblanc[6]	290 °K	− 15.9	+ 12.1	− 13.2	− 19.5	+ 5.02	+ 0.87
Katz *et al.*[7]							
	290 °K	− 20.71	15.63	− 18.35	− 24.82	4.15	0.67
Delacôte[8]	290 °K	− 22.3	16.75	− 18.2	− 24.60	4.52	0.80
	95 °K	− 23.2	17.05	− 25.85	− 33.10	5.95	0.732

However some of the values underlined in Table 1 published in (1) are strongly different from values reported by other authors. Those differences cannot be accounted by the previous arguments. We believe that those numbers should be revised.

The largest contribution to the temperature dependence of the mobility which can be deduced from corrected values of T.I. is in $T^{-0.6}$, which gives a maximum value of $n < 1.6$ in $\mu \alpha T^{-n}$. Therefore the values of n quoted in Table 5[1] are wrong in sign (a,b) and much too large (a,b,c') in magnitude for the holes, and too small in magnitude for the electrons. Almost all of the conclusions on the shape of the bands at 95 °K must also be revised, except Figs. 3 and 5[1] which figure out the shapes of the excess electron band in the a^{-1} and the b^{-1} direction at 95 °K and 290 °K.

Finally there is the special temperature dependence of the electron mobility in the c' direction which certainly cannot be explained by the variation of the related transfer integrals with temperature (despite an increase of this T.I. computed with SCF wave functions, when the temperature goes up[4]). It is believed that this mobility is a kind of phonon assisted mobility result which cannot be satisfactorily described by the application of a simple " band model " picture to the calculation of charge transport parameters.

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