ELECTRICAL CONDUCTION IN AROMATIC HYDROCARBONS

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PREFACE

Theoretical efforts to explain the electrical conduction in organic semiconductors on the basis of the applicability of band theory started only a decade ago with the first band structure calculation on anthracene by LeBlanc (1961, J.Chem.Phys. 35, 1275; 1962, ibid. 36, 1082). These calculations were based on the assumption that the electron-exchange interactions were large compared with the electron-phonon interactions, so that the carriers behaved as quasi-free particles occasionally scattered by phonons. However, Munn and Siebrand (1970, J.Chem.Phys.52, 6391; 1971, Disc.Faraday Soc.51, 17) have argued that for some crystallographic directions in organic semiconductors, there is a possibility of the electron-phonon interactions being of the same order of magnitude or even greater than the electron-exchange interactions.

Most of the experimental attempts at measuring the drift mobilities in organic solids ended in failure. This in many cases, was due to the wrong choice of crystal direction dictated by the shape of the available crystals.

The object of the present thesis is to provide enough theoretical data on electron-exchange interactions and carrier mobility anisotropies in a number of organic solids in the hope that:

i) by analogy with the results for anthracene (to which Munn-Siebrand theory seems to apply more closely than the conventional band theory) one can suggest the direction for a possible hopping transport;

ii) the mobility anisotropies will suggest the crystal directions for future mobility measurements and hence stimulate work on growth of oriented single crystals; and

iii) the calculated mobilities in conjunction with future experiments will provide a much clearer understanding of the transport in organic semiconductors.

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D.C. Singh

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