CHARGE TRANSPORT IN ORGANIC SEMICONDUCTORS: HETEROATOMIC AROMATIC HYDROCARBONS

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Thesis submitted to Indian Institute of Technology,
Delhi for partial fulfilment of the
Degree of Doctor of Philosophy
1973

ACKNOWLEDGEMENTS

The author wishes to express his deep sense of gratitude to Dr. S.C. Mathur for his valuable guidance and enlightened discussions failing which the present work would have been nigh impossible. To Professor M.S. Sodha, the author would like to express his indebtedness for the encouragement and wise counsel, he has received, in so abundant a measure, throughout the period of the investigation.

The author is grateful to Professor K.L. Chopra, Head of the Physics Department, for providing all the facilities required for the execution of this work. The keen interest of Dr. B.B. Tripathi, Dr. D.P. Tewari and Dr. D.C. Dube in the work is also sincerely acknowledged.

With great pleasure, the author expresses his sincere thanks to Dr. D.C. Singh, Dr. Jai Singh and Dr. H.C. Gupta for fruitful discussions and to his colleagues and friends for their cooperation. Thanks are also due to Mr. N.S. Gupta for drawing the figures and to Mr. V.N. Sharma for an efficient typing.

Financial assistance from the Council of Scientific and Industrial Research, New Delhi, India and the computer facilities provided by the Director, Computer Centre of Delhi University, are acknowledged most gratefully.

Last but not the least, the love and inspiration rendered to the author by his sister Dr.(Miss) Jyoti Kamal, Mami and Mama and other well wishers are beyond words.

Object of the Thesis

Importance of understanding the conduction mechanism in organic semiconductors, before its industrial applications are possible, is well known. One of the most important factors, effecting the conduction, is charge carrier transport. The work for the present thesis was started with a view to investigate the effect of heteroatoms (nitrogen and oxygen) on the mobility of electrons and holes. In hydrocarbons, the electron-exchange interactions (E-E I) depend on transfer integrals between carbon atoms at neighbouring molecules. Since the spread of $2p_{\pi}$ orbitals is different for carbon, nitrogen and oxygen, it was thought that the presence of heteroatoms in a molecule in place of or in addition to carbon atoms should systematically effect E-E I. Also, because E-E I is known to effect the electron transport, it was felt that such a study may yield valuable information on the effect of heteroatoms on charge carrier mobilities. It was decided to investigate the applicability of band model and then do energy band structure and mobility calculations on a few heteroatomic molecular crystals and hence to calculate the carrier mobilities.

When the work was started a controversy was going on regarding the mobility of electron in c'($\perp$ ab) direction of anthracene. It was being argued that the change in crystal parameters with temperature may account for the variation of mobility. However, the results were not convincing. Therefore, it was decided to investigate theoretically the carrier mobilities in anthraquinone for which crystal parameters at five different temperatures are available.

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TABLES 4.1 - 4.20