

CHARGE TRANSPORT IN ORGANIC SEMICONDUCTORS:
HETEROATOMIC AROMATIC HYDROCARBONS

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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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