CHAPTER IV

RESULTS AND DISCUSSION

4.1 Results.

From equation (III.41), we get

$$G_o = \frac{(c + 1) \pm 2\sqrt{c}}{V(c - 1)^2}$$

The $\pm$ plus or minus sign in the above equation implies that there are two values of the Green's function for every value of c. These values of G_o are the values of the end points of the cut in the energy complex planes. This corresponds to the bandwidths of the impurity band. The density of states which is used to compute Green's function are obtained from Hong and Kopelman[18] and are reliable for very low concentration of c. The concentrations 'c' which we are interested are in low range, i.e, there between 0.001 to 0.09. The system which we will be studying is $C_{10}D_8/C_{10}H_8$, with $C_{10}D_8$ being the host and $C_{10}H_8$ being the guests.

For every value of concentrations 'c' in low range between 0.001 to 0.09. We get the energy bandwidths as shown in the figure 3.2 The values of energy bandwidths ΔE lie on the vertical axis and concentration 'c' lie on the horizontal axis. Curve I corresponds to this computation and Curve II corresponds to prediction of Hoshen and Jortner.

The prediction obtained by Hoshen and Jortner were obtained by using the form $\Delta E = \Delta\sqrt{c(1-c)}$

when ΔE = energy bandwidth

Δ = $\varepsilon_A - \varepsilon_B$

= trap depth

= 115 cm^{-1}

c = concentration of impurity or guest

The numerical datas of the two curves are shown in the table I, II and III. Table I lists this computation which gives the values of concentrations 'c' and G_o ; Table II gives the values of concentrations 'c' and ΔE while table III belongs to Hoshen and Jortner which gives the values of concentration 'c' and ΔE ,

4,2 Discussion.

The results of computations are for the range of very low concentrations of 'c' where $C_{10}D_8$ to be host and $C_{10}H_8$ to be guest. Curve I is the result of this computation which used approximation method as convergent method. Curve II belongs to Hoshen and Jortner which used the Coherent Potential Approximation or CPA. From the figure 3.2, we see that the convergent method does not differ too much from CPA method, The convergent method gives lower values than CPA method.

Curve II is rather smooth curve when compared with curve I

since the values of G_o used to compute for values of energy band-widths ΔE take from the work of Suporn who extrapolated the values of $G_o(E)$ from a figure. The 'G_o' of Suporn are not exact values,