CHAPTER IV

NUMERICAL TECHNIQUES

4.1 Introduction

In the previous chapter, we obtained the expression for the monomer self energy Σ_1

$$\Sigma_1 = c\Delta \left\{ \frac{1 + c\,\Delta\, G_o}{1 - (1 - 2c)\Delta\, G_o} \right\} \qquad (4.1.1)$$

The pole or singularity is determined by the zero of $\{1 - (1 - 2c)\ \Delta\ G_o\}$ or

$$\begin{aligned} 1 &= (1 - 2c)\ \Delta\ G_o \\ \frac{1}{(1 - 2c)\ \Delta} &= G_o \\ &= \int \frac{\rho_o(E')\ dE'}{E - E'} \end{aligned} \qquad (4.1.2)$$

which corresponds to Hong and Kopelman's[7] result when $c \longrightarrow o$.
In this chapter we will evaluate the relation between the monomer energies (E) and the reciprocal trap depth ($1/\Delta$) at the concentrations c = 0.0, 0.2, 0.4, 0.6, 0.8 and 1.0. In determining the value of the diagonal density of states function $\rho_o(E')$, we will take the exciton dispersion relation to be given by[7]

$$E(\vec{k}^{+}) = 2M_a \cos(\vec{k}.\vec{a}) + 2M_b \cos(\vec{k}.\vec{b}) + 2M_c \cos(\vec{k}.\vec{c})$$
$$+ 2M_{a+c}\{\cos(\vec{k}.\vec{a})\cos(\vec{k}.\vec{c}) - \sin(\vec{k}.\vec{a})\sin(\vec{k}.\vec{c})\}$$
$$\pm\Big[4M_{12}\cos\{\vec{k}.(\tfrac{\vec{a}}{2})\}\cos\{\vec{k}.(\tfrac{\vec{b}}{2})\} + 4M_{12}'\cos(\vec{k}.\vec{c})$$
$$\times\cos\{\vec{k}.(\tfrac{\vec{a}}{2})\}\cos\{\vec{k}.(\tfrac{\vec{b}}{2})\} - \sin(\vec{k}.\vec{c})\sin\{\vec{k}.(\tfrac{\vec{a}}{2})\}$$
$$\times\cos\{\vec{k}.(\tfrac{\vec{b}}{2})\}\Big] \qquad (4.1.3)$$

where M_a, M_b, M_c, M_{a+c}, M_{12} and M_{12}' are pairwise interaction constants.

4.2 Determination of the Density of States

The interaction constants to be used in the energy dispersion relation can be found in reference 9 (in this research we use set 1 constants). We can obtain the density of states from the dispersion relation. A total of 512,000 points in the Brillouin zone were included in the calculation. We considered only the plus branch $\{E(\vec{k}^{+})\}$ [The numerical calculation was performed on a IBM 370/138 computer at the Computer Service Center , Chulalongkorn University] . From

$$\rho_o(E') = N^{-1} \sum_{\vec{k}^{+}} \delta\{E' - E(\vec{k}^{+})\} \qquad (4.2.1)$$

and by using with a 1 cm^{-1} mesh, we get the result of Table 4.2.1, as shown in Fig.4.2.1 . To eliminate the fluctuation we smooth the curve before integration.

Table 4.2.1 The density of states

No.	E' (interval) cm^{-1}	E' (mean) cm^{-1}	$\rho_o(E')$ real $\times 512{,}000^{-1}$	$\rho_o(E')$ approximate $\times 512{,}000^{-1}$
1	less than -84.0	-84.5	296	735.304355
2	-84.0 — -83.0	-83.5	824	859.454173
3	-83.0 — -82.0	-82.5	1072	977.130246
4	-82.0 — -81.0	-81.5	1280	1088.520239
5	-81.0 — -80.0	-80.5	1240	1193.811761
6	-80.0 — -79.0	-79.5	1384	1293.192451
7	-79.0 — -78.0	-78.5	1784	1386.849933
8	-78.0 — -77.0	-77.5	1744	1474.971855
9	-77.0 — -76.0	-76.5	1888	1557.745842
10	-76.0 — -75.0	-75.5	2048	1635.359525
11	-75.0 — -74.0	-74.5	1752	1708.000536
12	-74.0 — -73.0	-73.5	1872	1775.856492
13	-73.0 — -72.0	-72.5	2208	1839.115056
14	-72.0 — -71.0	-71.5	1808	1897.963836
15	-71.0 — -70.0	-70.5	2032	1952.590473
16	-70.0 — -69.0	-69.5	1888	2003.182599
17	-69.0 — -68.0	-68.5	2152	2049.927838
18	-68.0 — -67.0	-67.5	1976	2093.013836
19	-67.0 — -66.0	-66.5	2112	2132.628219
20	-66.0 — -65.0	-65.5	1968	2168.958611
21	-65.0 — -64.0	-64.5	2048	2202.192659
22	-64.0 — -63.0	-63.5	2392	2232.517974

No.	E' (interval) cm^{-1}	E' (mean) cm^{-1}	$\rho_o(E')$ real $\times 512{,}000^{-1}$	$\rho_o(E')$ approximate $\times 512{,}000^{-1}$
23	-63.0 — -62.0	-62.5	1992	2260.122208
24	-62.0 — -61.0	-61.5	1936	2285.192987
25	-61.0 — -60.0	-60.5	2104	2207.917943
26	-60.0 — -59.0	-59.5	2288	2328.484707
27	-59.0 — -58.0	-58.5	2288	2347.080906
28	-58.0 — -57.0	-57.5	2272	2363.894183
29	-57.0 — -56.0	-56.5	2064	2379.112160
30	-56.0 — -55.0	-55.5	2168	2392.922479
31	-55.0 — -54.0	-54.5	2368	2405.512755
32	-54.0 — -53.0	-53.5	2312	2417.070643
33	-53.0 — -52.0	-52.5	2368	2427.783759
34	-52.0 — -51.0	-51.5	2208	2437.839734
35	-51.0 — -50.0	-50.5	2288	2447.426211
36	-50.0 — -49.0	-49.5	2400	2456.730812
37	-49.0 — -48.0	-48.5	2536	2465.941179
38	-48.0 — -47.0	-47.5	2384	2475.244934
39	-47.0 — -46.0	-46.5	2416	2484.829719
40	-46.0 — -45.0	-45.5	2296	2494.883155
41	-45.0 — -44.0	-44.5	2480	2505.592877
42	-44.0 — -43.0	-43.5	2536	2517.146526
43	-43.0 — -42.0	-42.5	2648	2529.731724
44	-42.0 — -41.0	-41.5	2568	2543.536109

No.	E' (interval) cm^{-1}	E' (mean) cm^{-1}	$\rho_o(E')$ real $\times 512{,}000^{-1}$	$\rho_o(E')$ approximate $\times 512{,}000^{-1}$
45	-41.0 — -40.0	-40.5	2504	2558.747307
46	-40.0 — -39.0	-39.5	2496	2575.552954
47	-39.0 — -38.0	-38.5	2720	2594.140686
48	-38.0 — -37.0	-37.5	2936	2614.698127
49	-37.0 — -36.0	-36.5	2576	2637.412914
50	-36.0 — -35.0	-35.5	2648	2662.472678
51	-35.0 — -34.0	-34.5	2600	2690.065051
52	-34.0 — -33.0	-33.5	3008	2720.377661
53	-33.0 — -32.0	-32.5	3040	2753.598149
54	-32.0 — -31.0	-31.5	2832	2789.914142
55	-31.0 — -30.0	-30.5	2792	2829.513269
56	-30.0 — -29.0	-29.5	2952	2872.583165
57	-29.0 — -28.0	-28.5	2912	2919.311462
58	-28.0 — -27.0	-27.5	3256	2969.885793
59	-27.0 — -26.0	-26.5	3264	3024.493790
60	-26.0 — -25.0	-25.5	2840	3083.323084
61	-25.0 — -24.0	-24.5	3296	3146.561305
62	-24.0 — -23.0	-23.5	2912	3214.396089
63	-23.0 — -22.0	-22.5	3464	3287.015065
64	-22.0 — -21.0	-21.5	3680	3364.605869
65	-21.0 — -20.0	-20.5	3216	3447.356128
66	-20.0 — -19.0	-19.5	3376	3535.453476

No.	E' (interval) cm^{-1}	E' (mean) cm^{-1}	$\rho_o(E')$ real $\times 512{,}000^{-1}$	$\rho_o(E')$ approximate $\times 512{,}000^{-1}$
67	-19.0 — -18.0	-18.5	3672	3629.085547
68	-18.0 — -17.0	-17.5	3656	3728.439970
69	-17.0 — -16.0	-16.5	3384	3833.704378
70	-16.0 — -15.0	-15.5	4032	3945.066405
71	-15.0 — -14.0	-14.5	4072	4062.713681
72	-14.0 — -13.0	-13.5	4208	4186.833839
73	-13.0 — -12.0	-12.5	4016	4317.614510
74	-12.0 — -11.0	-11.5	4096	4455.243326
75	-11.0 — -10.0	-10.5	4848	4599.907921
76	-10.0 — - 9.0	- 9.5	4808	4751.795925
77	- 9.0 — - 8.0	- 8.5	5216	{ 4911 094971 4876.101301 }
78	- 8.0 — - 7.0	- 7.5	4576	4868.916533
79	- 7.0 — - 6.0	- 6.5	4944	4862.874157
80	- 6.0 — - 5.0	- 5.5	4608	4857.967664
81	- 5.0 — - 4.0	- 4.5	4656	4864.190547
82	- 4.0 — - 3.0	- 3.5	5104	351.536298
83	- 3.0 — - 2.0	- 2.5	4912	4849.998408
84	- 2.0 — - 1.0	- 1.5	4736	4849.570371
85	- 1.0 — 0.0	- 0.5	4768	4850.245677
86	0.0 — 1.0	0.5	5040	4852.017819
87	1.0 — 2.0	1.5	4920	4854.880287
88	2.0 — 3.0	2.5	4856	4858.826579

No.	E' (interval) cm^{-1}	E' (mean) cm^{-1}	$\rho_o(E')$ real x 512,000	$\rho_o(E')$ approximate x 512,000
89	3.0. — 4.0	3.5	4848	4863.850181
90	4.0 — 5.0	4.5	4528	4869.944587
91	5.0 — 6.0	5.5	5464	4877.103290
92	6.0 — 7.0	6.5	4840	4885.319780
93	7.0 — 8.0	7.5	5000	4894.587551
94	8.0 — 9.0	8.5	4752	4904.900094
95	9.0 — 10.0	9.5	4840	4916.250902
96	10.0 — 11.0	10.5	5088	4928.633465
97	11.0 — 12.0	11.5	5048	4942.041278
98	12.0 — 13.0	12.5	4856	4956.467831
99	13.0 — 14.0	13.5	4896	4971.906616
100	14.0 — 15.0	14.5	4960	4988.351126
101	15.0 — 16.0	15.5	5208	5005.794852
102	16.0 — 17.0	16.5	5000	5024.231287
103	17.0 — 18.0	17.5	4944	5043.653923
104	18.0 — 19.0	18.5	5168	5064.056252
105	19.0 — 20.0	19.5	5036	5085.431765
106	20.0 — 21.0	20.5	5052	5107.773955
107	21.0 — 22.0	21.5	5392	5131.076314
108	22.0 — 23.0	22.5	4712	5155.332334
109	23.0 — 24.0	23.5	5072	5180.535507
110	24.0 — 25.0	24.5	5496	{ 5206.679325 5285.384362 }

No.	E' (interval) cm^{-1}	E' (mean) cm^{-1}	$\rho_o(E')$ real $\times 512{,}000^{-1}$	$\rho_o(E')$ approximate $\times 512{,}000^{-1}$
111	25.0 — 26.0	25.5	5120	5182.698796
112	26.0 — 27.0	26.5	5088	5082.240821
113	27.0 — 28.0	27.5	5208	4983.885027
114	28.0 — 29.0	28.5	4960	4887.506004
115	29.0 — 30.0	29.5	4896	4792.978344
116	30.0 — 31.0	30.5	4824	4700.176635
117	31.0 — 32.0	31.5	4392	4608.975466
118	32.0 — 33.0	32.5	3980	4519.249428
119	33.0 — 34.0	33.5	4540	4430.873109
120	34.0 — 35.0	34.5	3936	4343.721103
121	35.0 — 36.0	35.5	4072	4257.667997
122	36.0 — 37.0	36.5	4528	4172.588381
123	37.0 — 38.0	37.5	3536	4088.356843
124	38.0 — 39.0	38.5	3752	4004.847979
125	39.0 — 40.0	39.5	4136	3921.936374
126	40.0 — 41.0	40.5	3920	3839.496618
127	41.0 — 42.0	41.5	3664	3757.403300
128	42.0 — 43.0	42.5	3320	3675.531011
129	43.0 — 44.0	43.5	3848	3593.754345
130	44.0 — 45.0	44.5	4032	3511.947882
131	45.0 — 46.0	45.5	3436	3429.986222
132	46.0 — 47.0	46.5	3444	3347.743950

No.	E' (interval) cm^{-1}	E' (mean) cm^{-1}	$\rho_o(E')$ real $\times 512{,}000^{-1}$	$\rho_o(E')$ approximate $\times 512{,}000^{-1}$
133	47.0 — 48.0	47.5	3448	3265.095660
134	48.0 — 49.0	48.5	3808	3181.915938
135	49.0 — 50.0	49.5	3384	3098.079369
136	50.0 — 51.0	50.5	3096	3013.460556
137	51.0 — 52.0	51.5	2928	2927.934076
138	52.0 — 53.0	52.5	3152	2841.374523
139	53.0 — 54.0	53.5	2616	2753.656492
140	54.0 — 55.0	54.5	2336	2664.654567
141	55.0 — 56.0	55.5	3512	2574.243339
142	56.0 — 57.0	56.5	2448	2482.297398
143	57.0 — 58.0	57.5	2336	2388.691338
144	58.0 — 59.0	58.5	1888	2293.299744
145	59.0 — 60.0	59.5	2216	2195.997200
146	60.0 — 61.0	60.5	1976	2096.658314
147	61.0 — 62.0	61.5	1728	1995.157657
148	62.0 — 63.0	62.5	1920	1891.369832
149	63.0 — 64.0	63.5	1664	1785.169422
150	64.0 — 65.0	64.5	1584	1676.431011
151	65.0 — 66.0	65.5	1552	1565.029208
152	66.0 — 67.0	66.5	1344	1450.838583
153	67.0 — 68.0	67.5	1384	1333.733739
154	68.0 — 69.0	68.5	1320	1213.589260

No.	E' (interval) cm^{-1}	E' (mean) cm^{-1}	$\rho_o(E')$ real $\times 512{,}000^{-1}$	$\rho_o(E')$ approximate $\times 512{,}000^{-1}$
155	69.0 — 70.0	69.5	1112	1090.279728
156	70.0 — 71.0	70.5	1064	963.679754
157	71.0 — 72.0	71.5	912	833.663914
158	72.0 — 73.0	72.5	856	700.106790
159	73.0 — 74.0	73.5	688	562.882988
160	74.0 — 75.0	74.5	496	421.867089
161	greater than 75.0	75.5	264	276.933691

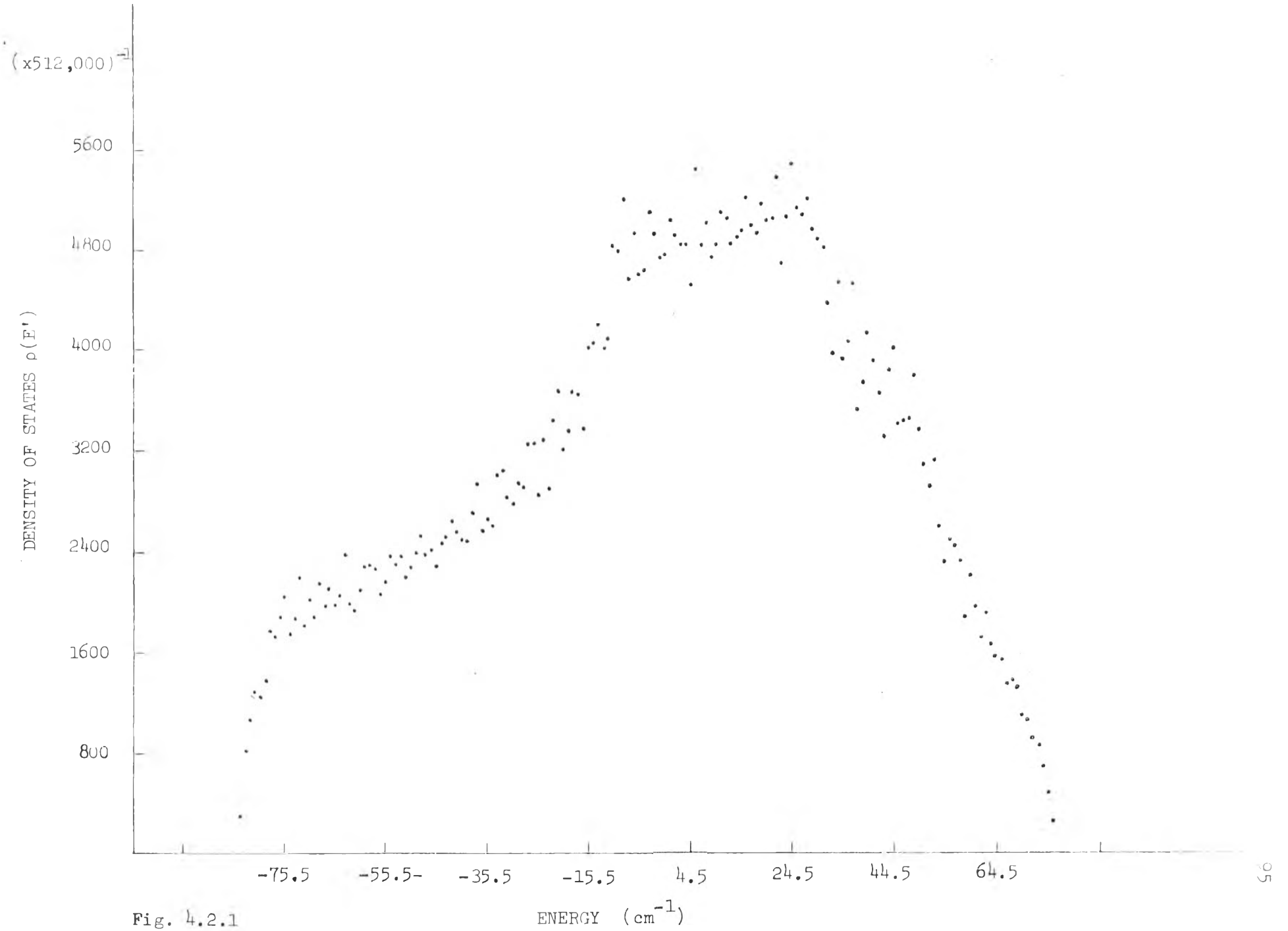

(x512,000)$^{-1}$
5600
4800
4000
3200
2400
1600
800
DENSITY OF STATES ρ(E')
-75.5
-55.5-
-35.5
-15.5
4.5
24.5
44.5
64.5
ENERGY (cm^{-1})

Fig. 4.2.1

4.3 The Method of Least Squares for Curve Fitting[26]

This method says that the best representative curve is that for which the sum of the squares of the residuals is a minimum. Since the squares of the residuals are positive quantities, the requirement that their sum be as small as possible ensures that the numerical values of the residuals will be small.

Let us consider the formula

$$y = a + bx + cx^2 + dx^3 \qquad (4.3.1)$$

the task is then to find the values of a, b, c, and d which will make the graph of (4.3.1) pass as near as possible to each of the n points (x_1, y_1) , (x_2 , y_2) ,..., (x_n , y_n); or in other words, we must find an equation of the form (4.3.1) which will be satisfied as nearly as possible by each of the n pairs of observed values (x_1 , y_1) , (x_2 , y_2), ...,(x_n , y_n). The equation will not, in general, be satisfied exactly by any of the n pairs. Substituting in (4.3.1) each of the n pairs of values in turn, we get the following residual equations:

$$\begin{aligned} v_1 &= a + bx_1 + cx_1^2 + dx_1^3 - y_1 \ , \\ v_2 &= a + bx_2 + cx_2^2 + dx_2^3 - y_2 \ , \\ &\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ v_n &= a + bx_n + cx_n^2 + dx_n^3 - y_n \end{aligned} \qquad (4.3.2)$$

The principle of least squares says that the best values of the unknown constants a, b, c, and d are those which make the sum of the squares of the residuals a minimum, or

$$\Sigma v^2 = v_1^2 + v_2^2 + v_3^2 + \ldots + v_n^2 \qquad (4.3.3)$$

must be a minimum. Hence

$$\begin{aligned}\Sigma (a + bx + cx^2 + dx^3 - y)^2 &= (a + bx_1 + cx_1^2 + dx_1^3 - y_1)^2 \\ &\quad +(a + bx_2 + cx_2^2 + dx_2^3 - y_2)^2 \\ &\quad + \ldots \\ &\quad +(a + bx_n + cx_n^2 + dx_n^3 - y_n)^2 \\ &= f(a, b, c, d) \qquad (4.3.4)\end{aligned}$$

is to be a minimum

The condition that f(a, b, c, d) be a maximum or minimum is that its partial derivatives with respect to a, b, c, and d will each be zero. We therefore have

$$\begin{aligned}\frac{\partial f}{\partial a} &= 2(a + bx_1 + cx_1^2 + dx_1^3 - y_1) + 2(a + bx_2 + cx_2^2 + dx_2^3 - y_2) + \ldots = 0 \\ \frac{\partial f}{\partial b} &= 2(a + bx_1 + cx_1^2 + dx_1^3 - y_1)x_1 + 2(a + bx_2 + cx_2^2 + dx_2^3 - y_2)x_2 + \ldots = 0 \\ \frac{\partial f}{\partial c} &= 2(a + bx_1 + cx_1^2 + dx_1^3 - y_1)x_1^2 + 2(a + bx_2 + cx_2^2 + dx_2^3 - y_2)x_2^2 + \ldots = 0 \\ \frac{\partial f}{\partial d} &= 2(a + bx_1 + cx_1^2 + dx_1^3 - y_1)x_1^3 + 2(a + bx_2 + cx_2^2 + dx_2^3 - y_2)x_2^3 + \ldots = 0\end{aligned} \qquad (4.3.5)$$

Dividing through (4.3.5) by 2 , we get the following four normal equations :

$$(a+bx_1+cx_1^2+dx_1^3-y_1)+(a+bx_2+cx_2^2+dx_2^3-y_2)+..+(a+bx_n+cx^2_n+dx^3_n-y_n) \quad =0$$

$$x_1(a+bx_1+cx_1^2+dx_1^3-y_1)+x_2(a+bx_2+cx_2^2+dx_2^3-y_2)+...+x_n(a+bx_n+cx_n^2+dx_n^3-y_n)=0$$

$$x_1^2(a+bx_1+cx_1^2+dx_1^3-y_1)+x_2^2(a+bx_2+cx_2^2+dx_2^3-y_2)+...+x_n^2(a+bx_n+cx_n^2+dx_n^3-y_n)=0$$

$$x_1^3(a+bx_1+cx_1^2+dx_1^3-y_1)+x_2^3(a+bx_2+cx_2^2+dx_2^3-y_2)+...+x_n^2(a+bx_n+cx_n^2+dx_n^3-y_n)=0$$

(4.3.6)

Simplify (4.3.6) , we will get the system of linear algebraic equations,

$$a\sum_{i=1}^{n} x_i^0 + b\sum_{i=1}^{n} x_i \quad c\sum_{i=1}^{n} x_i^2 + d\sum_{i=1}^{n} x_i^3 = \sum_{i=1}^{n} y_i$$

$$a\sum_{i=1}^{n} x_i + b\sum_{i=1}^{n} x_i^2 + c\sum_{i=1}^{n} x_i^3 + d\sum_{i=1}^{n} x_i^4 = \sum_{i=1}^{n} x_i y_i$$

$$a\sum_{i=1}^{n} x_i^2 + b\sum_{i=1}^{n} x_i^3 + c\sum_{i=1}^{n} x_i^4 + d\sum_{i=1}^{n} x_i^5 = \sum_{i=1}^{n} x_i^2 y_i$$

$$a\sum_{i=1}^{n} x_i^3 + b\sum_{i=1}^{n} x_i^4 + c\sum_{i=1}^{n} x_i^5 + d\sum_{i=1}^{n} x_i^6 = \sum_{i=1}^{n} x_i^3 y_i$$

(4.3.7)

The system of linear equations of (4.3.7) is often written in matrix form as

$$\begin{bmatrix} \Sigma x_i^0 & \Sigma x_i & \Sigma x_i^2 & \Sigma x_i^3 \\ \Sigma x_i & \Sigma x_i^2 & \Sigma x_i^3 & \Sigma x_i^4 \\ \Sigma x_i^2 & \Sigma x_i^3 & \Sigma x_i^4 & \Sigma x_i^5 \\ \Sigma x_i^3 & \Sigma x_i^4 & \Sigma x_i^5 & \Sigma x_i^6 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = \begin{bmatrix} \Sigma y_i \\ \Sigma x_i y_i \\ \Sigma x_i^2 y_i \\ \Sigma x_i^3 y_i \end{bmatrix} \tag{4.3.8}$$

We must divided the domain E' of $\rho_o(E')$ into three parts, shown in Fig.4.2.1, since the density of states appears to have a different functional dependence in the three domains. So we will have three formula like (4.3.1) but different a, b, c, and d in each domains. In calculation a, b, c, and d in three domains and familiar curve fitting calculation, we performed on a Hewlett - Packard 97 Programmable Printing Calculator of Department of Physics, Chulalongkorn University. The result as shown in Table 4.2.1 and plot graph shown in Fig.4.3.1 (solid curve). The values of a, b, c, and d shown in Table 4.3.1

We must evaluate the curve intersection points ; P_1, P_2, P_3 and P_4 as shown in Fig.4.3.1. This calculation was performed on a Hewlett - Packard 97 Programmable Calculator. The results are shown in Table 4.3.2

Table 4.3.1 The values of a, b, c, and d in three domains

domains	a	b	c	d
1	6590.872421	234.43404480	4.5967730250	0.0312720057 90
2	4850.995050	1.7724132500	0.5467909725	-.0010846589 78
3	8843.070426	-199.1284256	2.7127750440	-.0209016893 90

Table 4.3.2 The curve intersection points

P_1	=	-89.566617220
P_2	=	- 8.705647419
P_3	=	25.105279050
P_4	=	77.337419820

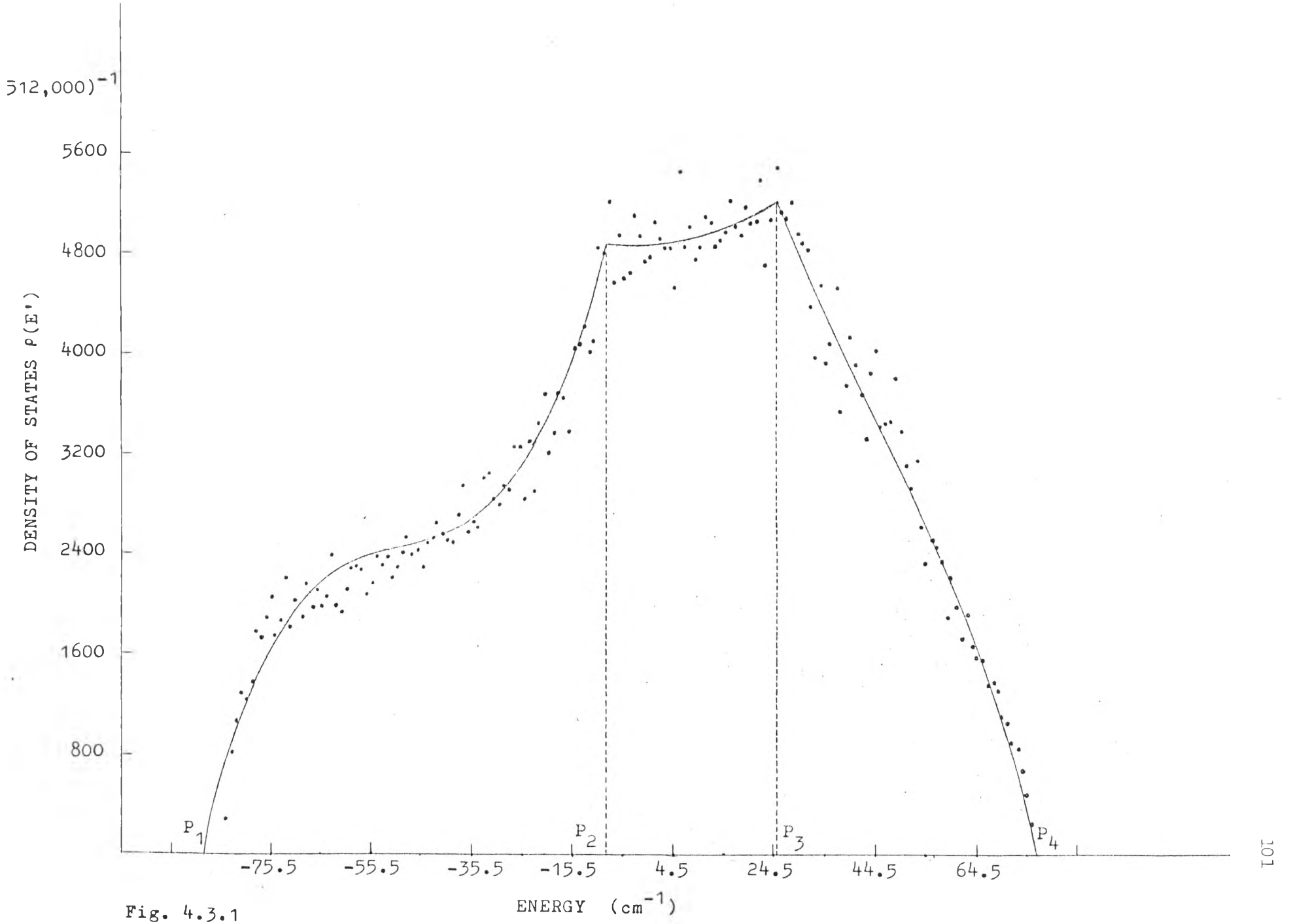

512,000)^-1
5600
4800
4000
3200
2400
1600
800
DENSITY OF STATES ρ(E')
P1
P2
P3
P4
-75.5
-55.5
-35.5
-15.5
4.5
24.5
44.5
64.5
ENERGY (cm^-1)

Fig. 4.3.1

4.4 Determination of $\int \{\rho_o(E')/(E - E')\}\ dE'$

In our calculation, we have used $\rho_o(E')$ from section 4.3 and proceed by parts. We begin with E equal to -150, increasing E by 1 at each iteration until the value of E equal to 150. For each E we check to see whether E is inside the energy interval spanned by the density of states. If it is, we separate the integral as follows

$$\int_{\text{left edge}}^{\text{right edge}} \{\rho_o(E')/(E - E')\}\ dE' = \int_{\text{left edge}}^{E - \delta} \{\rho_o(E')/(E - E')\}\ dE' + \int_{E + \delta}^{\text{right edge}} \{\rho(E')/(E - E')\}\ dE' \qquad (4.4.1)$$

and calculate each of them by the Newton - Cotes open type 5 points method[27]. If E is not within the density of states energy band we proceed to evaluate the integral directly

The integration formulas are obtained by dividing the interval (a, b) into n equal parts by inserting n-1 equally spaced interior abscissas, then approximating $f(x)\{$ in our calculation $f(x) = f(E') = \rho_o(E')/(E - E')\}$ by the polynomial of degree n-2 which coincides with f(x) at the n-1 interior points, and approximating the relevant integral by integrating the resultant polynomial over (a,b). These formulas thus do not involve the ordinates at the ends of the interval and

said to be of open type. For the case n = 6, the formula may be expressed as follows :

$$\int_{x_0}^{x_6} f(x)\,dx = \frac{3h}{10}(11f_1 - 14f_2 + 26f_3 - 14f_4 + 11f_5) + \frac{41}{140}h^7 f^{vi}(\xi)$$

where $x_0 < \xi < x_6$ (4.4.2)

After integration is successful, we can evaluate the relation between $1/\Delta$ and E at various concentration range from (4.1.2). The results shown as in Table 4.4.1 and in Fig.4.4.1 a-f This calculation was performed on a IBM 370/138 Computer at the Computer Service Center, Chulalongkorn University.

Table 4.4.1 The monomer energies and the reciprocal trap depth ($\times 512{,}000^{-1}$ cm) at c = 0.0, 0.2, 0.4, 0.6, 0.8, 1.0

THE RECIPROCAL TRAP DEPTH

I	E	C=0.0	C=0.2	C=0.4	C=0.6	C=0.8	C=1.0
1	-150.00	-3718.306169	-2230.983568	-743.661189	743.661189	2230.983568	3718.306169
2	-149.00	-3748.194279	-2248.916433	-749.638811	749.638811	2248.916433	3748.194279
3	-148.00	-3778.622935	-2267.173626	-755.724542	755.724542	2267.173626	3778.622935
4	-147.00	-3809.608648	-2285.765053	-761.921684	761.921684	2285.765053	3809.608648
5	-146.00	-3841.168678	-2304.701069	-768.233690	768.233690	2304.701069	3841.168678
6	-145.00	-3873.321078	-2323.992508	-774.664169	774.664169	2323.992508	3873.321078
7	-144.00	-3906.084749	-2343.650710	-781.216903	781.216903	2343.650710	3906.084749
8	-143.00	-3939.479491	-2363.687554	-787.895851	787.895851	2363.687554	3939.479491
9	-142.00	-3973.526063	-2384.115496	-794.705165	794.705165	2384.115496	3973.526063
10	-141.00	-4008.246247	-2404.947605	-801.649202	801.649202	2404.947605	4008.246247
11	-140.00	-4043.662916	-2426.197605	-808.732535	808.732535	2426.197605	4043.662916
12	-139.00	-4079.800113	-2447.879922	-815.959974	815.959974	2447.879922	4079.800113
13	-138.00	-4116.683128	-2470.009729	-823.336576	823.336576	2470.009729	4116.683128
14	-137.00	-4154.338591	-2492.603006	-830.867669	830.867669	2492.603006	4154.338591
15	-136.00	-4192.794572	-2515.676593	-838.558864	838.558864	2515.676593	4192.794572
16	-135.00	-4232.080683	-2539.248259	-846.416086	846.416086	2539.248259	4232.080683
17	-134.00	-4272.228202	-2563.336769	-854.445590	854.445590	2563.336769	4272.228202
18	-133.00	-4313.270198	-2587.961964	-862.653988	862.653988	2587.961964	4313.270198
19	-132.00	-4355.241675	-2613.144849	-871.048283	871.048283	2613.144849	4355.241675
20	-131.00	-4398.179732	-2638.907682	-879.635894	879.635894	2638.907682	4398.179732
21	-130.00	-4442.123735	-2665.274082	-888.424694	888.424694	2665.274082	4442.123735
22	-129.00	-4487.115512	-2692.269147	-897.423049	897.423049	2692.269147	4487.115512
23	-128.00	-4533.199568	-2719.919579	-906.639860	906.639860	2719.919579	4533.199568
24	-127.00	-4580.423324	-2748.253831	-916.084610	916.084610	2748.253831	4580.423324
25	-126.00	-4628.837386	-2777.302266	-925.767422	925.767422	2777.302266	4628.837386
26	-125.00	-4678.495843	-2807.097339	-935.699113	935.699113	2807.097339	4678.495843
27	-124.00	-4729.456612	-2837.673798	-945.891266	945.891266	2837.673798	4729.456612
28	-123.00	-4781.781809	-2869.068915	-956.356305	956.356305	2869.068915	4781.781809
29	-122.00	-4835.538188	-2901.322740	-967.107580	967.107580	2901.322740	4835.538188
30	-121.00	-4890.797626	-2934.478400	-978.159467	978.159467	2934.478400	4890.797626
31	-120.00	-4947.637681	-2968.582432	-989.527477	989.527477	2968.582432	4947.637681
32	-119.00	-5006.142234	-3003.685161	-1001.228387	1001.228387	3003.685161	5006.142234
33	-118.00	-5066.402217	-3039.841149	-1013.280383	1013.280383	3039.841149	5066.402217
34	-117.00	-5128.516463	-3077.109694	-1025.703231	1025.703231	3077.109694	5128.516463
35	-116.00	-5192.592688	-3115.555427	-1038.518476	1038.518476	3115.555427	5192.592688
36	-115.00	-5258.748634	-3155.248992	-1051.749664	1051.749664	3155.248992	5258.748634
37	-114.00	-5327.113413	-3196.267858	-1065.422619	1065.422619	3196.267858	5327.113413
38	-113.00	-5397.829091	-3238.697262	-1079.565754	1079.565754	3238.697262	5397.829091
39	-112.00	-5471.052567	-3282.631345	-1094.210448	1094.210448	3282.631345	5471.052567
40	-111.00	-5546.957825	-3328.174497	-1109.391499	1109.391499	3328.174497	5546.957825
41	-110.00	-5625.738642	-3375.442984	-1125.147661	1125.147661	3375.442984	5625.738642
42	-109.00	-5707.611884	-3424.566926	-1141.522309	1141.522309	3424.566926	5707.611884
43	-108.00	-5792.821550	-3475.692723	-1158.564241	1158.564241	3475.692723	5792.821550
44	-107.00	-5881.643781	-3528.986058	-1176.328686	1176.328686	3528.986058	5881.643781
45	-106.00	-5974.393144	-3584.635673	-1194.878558	1194.878558	3584.635673	5974.393144
46	-105.00	-6071.430608	-3642.858147	-1214.286049	1214.286049	3642.858147	6071.430608
47	-104.00	-6173.173818	-3703.904070	-1234.634690	1234.634690	3703.904070	6173.173818
48	-103.00	-6280.110540	-3768.066099	-1256.022033	1256.022033	3768.066099	6280.110540
49	-102.00	-6392.816564	-3835.689710	-1278.563237	1278.563237	3835.689710	6392.816564
50	-101.00	-6511.980058	-3907.187802	-1302.395934	1302.395934	3907.187802	6511.980058

THE RECIPROCAL TRAP DEPTH

I	C	C=0.0	C=0.2	C=0.4	C=0.6	C=0.8	C=1.0
51	-100.00	-6638.435445	-3983.061029	-1327.687010	1327.687010	3983.061029	6638.435445
52	-99.00	-6773.211822	-4063.926851	-1354.642284	1354.642284	4063.926851	6773.211822
53	-98.00	-6917.604319	-4150.562344	-1383.520781	1383.520781	4150.562344	6917.604319
54	-97.00	-7073.283051	-4243.969573	-1414.656526	1414.656526	4243.969573	7073.283051
55	-96.00	-7242.466563	-4345.479679	-1448.493226	1448.493226	4345.479679	7242.466563
56	-95.00	-7428.211726	-4456.926770	-1485.642257	1485.642257	4456.926770	7428.211726
57	-94.00	-7634.927219	-4580.956058	-1526.985353	1526.985353	4580.956058	7634.927219
58	-93.00	-7869.348777	-4721.608985	-1573.869662	1573.869662	4721.608985	7869.348777
59	-92.00	-8142.557001	-4885.533910	-1628.511303	1628.511303	4885.533910	8142.557001
60	-91.00	-8474.628426	-5084.776752	-1694.925584	1694.925584	5084.776752	8474.628426
61	-90.00	-8906.995676	-5344.197087	-1781.399029	1781.399029	5344.197087	8906.995676
62	-89.00	-9444.348306	-5666.608646	-1888.869549	1888.869549	5666.608646	9444.348306
63	-88.00	-9806.577095	-5883.945906	-1961.315302	1961.315302	5883.945906	9806.577095
64	-87.00	-10037.757209	-6022.653966	-2007.551322	2007.551322	6022.653966	10037.757209
65	-86.00	-10184.507924	-6110.704390	-2036.901463	2036.901463	6110.704390	10184.507924
66	-85.00	-10271.657678	-6162.994240	-2054.331413	2054.331413	6162.994240	10271.657678
67	-84.00	-10313.987650	-6188.392221	-2062.797407	2062.797407	6188.392221	10313.987650
68	-83.00	-10321.133439	-6192.679694	-2064.226565	2064.226565	6192.679694	10321.133439
69	-82.00	-10299.858415	-6179.914680	-2059.971560	2059.971560	6179.914680	10299.858415
70	-81.00	-10255.200186	-6153.119745	-2051.039915	2051.039915	6153.119745	10255.200186
71	-80.00	-10191.090686	-6114.654047	-2038.218016	2038.218016	6114.654047	10191.090686
72	-79.00	-10110.712457	-6066.427137	-2022.142379	2022.142379	6066.427137	10110.712457
73	-78.00	-10016.714920	-6010.028594	-2003.342865	2003.342865	6010.028594	10016.714920
74	-77.00	-9911.351468	-5946.810526	-1982.270175	1982.270175	5946.810526	9911.351468
75	-76.00	-9796.571253	-5877.942402	-1959.314134	1959.314134	5877.942402	9796.571253
76	-75.00	-9674.082130	-5804.448932	-1934.816311	1934.816311	5804.448932	9674.082130
77	-74.00	-9545.395850	-5727.237168	-1909.079056	1909.079056	5727.237168	9545.395850
78	-73.00	-9411.861351	-5647.116474	-1882.372158	1882.372158	5647.116474	9411.861351
79	-72.00	-9274.689933	-5564.813628	-1854.937876	1854.937876	5564.813628	9274.689933
80	-71.00	-9134.974725	-5480.984509	-1826.994836	1826.994836	5480.984509	9134.974725
81	-70.00	-8993.706005	-5396.223281	-1798.741094	1798.741094	5396.223281	8993.706005
82	-69.00	-8851.783423	-5311.069737	-1770.356579	1770.356579	5311.069737	8851.783423
83	-68.00	-8710.025841	-5226.015193	-1742.005064	1742.005064	5226.015193	8710.025841
84	-67.00	-8569.179266	-5141.507253	-1713.835751	1713.835751	5141.507253	8569.179266
85	-66.00	-8429.923198	-5057.953618	-1685.984539	1685.984539	5057.953618	8429.923198
86	-65.00	-8292.875567	-4975.725044	-1658.575015	1658.575015	4975.725044	8292.875567
87	-64.00	-8158.596324	-4895.157503	-1631.719168	1631.719168	4895.157503	8158.596324
88	-63.00	-8027.589618	-4816.553484	-1605.517828	1605.517828	4816.553484	8027.589618
89	-62.00	-7900.304320	-4740.182310	-1580.060770	1580.060770	4740.182310	7900.304320
90	-61.00	-7777.132478	-4666.279209	-1555.426403	1555.426403	4666.279209	7777.132478
91	-60.00	-7658.404994	-4595.042723	-1531.680908	1531.680908	4595.042723	7658.404994
92	-59.00	-7544.383478	-4526.629817	-1508.876606	1508.876606	4526.629817	7544.383478
93	-58.00	-7435.246838	-4461.147837	-1487.049279	1487.049279	4461.147837	7435.246838
94	-57.00	-7331.071018	-4398.642349	-1466.214116	1466.214116	4398.642349	7331.071018
95	-56.00	-7231.801177	-4339.080447	-1446.360149	1446.360149	4339.080447	7231.801177
96	-55.00	-7137.220391	-4282.331980	-1427.443993	1427.443993	4282.331980	7137.220391
97	-54.00	-7046.936843	-4228.161853	-1409.387284	1409.387284	4228.161853	7046.936843
98	-53.00	-6960.472947	-4176.283519	-1392.094506	1392.094506	4176.283519	6960.472947
99	-52.00	-6877.754137	-4126.652236	-1375.550745	1375.550745	4126.652236	6877.754137
100	-51.00	-6801.087375	-4080.652182	-1360.217394	1360.217394	4080.652182	6801.087375

THE RECIPROCAL TRAP DEPTH

I	E	C=0.0	C=0.2	C=0.4	C=0.6	C=0.8	C=1.0
101	-50.00	-6742.990135	-4045.793840	-1348.597947	1348.597947	4045.793840	6742.990135
102	-49.00	-6756.139079	-4053.683206	-1351.227735	1351.227735	4053.683206	6756.139079
103	-48.00	-6750.028845	-4050.017066	-1350.005689	1350.005689	4050.017066	6750.028845
104	-47.00	-6706.390086	-4023.833812	-1341.277937	1341.277937	4023.833812	6706.390086
105	-46.00	-6662.599562	-3997.559499	-1332.519833	1332.519833	3997.559499	6662.599562
106	-45.00	-6626.793264	-3976.075722	-1325.358574	1325.358574	3976.075722	6626.793264
107	-44.00	-6600.113297	-3960.067742	-1320.022581	1320.022581	3960.067742	6600.113297
108	-43.00	-6582.049542	-3949.229490	-1316.409830	1316.409830	3949.229490	6582.049542
109	-42.00	-6571.814608	-3943.088530	-1314.362843	1314.362843	3943.088530	6571.814608
110	-41.00	-6568.677110	-3941.206031	-1313.735344	1313.735344	3941.206031	6568.677110
111	-40.00	-6572.011854	-3943.206877	-1314.402292	1314.402292	3943.206877	6572.011854
112	-39.00	-6581.278881	-3948.767093	-1316.255698	1316.255698	3948.767093	6581.278881
113	-38.00	-6595.991275	-3957.594529	-1319.198176	1319.198176	3957.594529	6595.991275
114	-37.00	-6615.687186	-3969.412075	-1323.137358	1323.137358	3969.412075	6615.687186
115	-36.00	-6639.908497	-3983.944861	-1327.981620	1327.981620	3983.944861	6639.908497
116	-35.00	-6668.185140	-4000.910846	-1333.636949	1333.636949	4000.910846	6668.185140
117	-34.00	-6700.023480	-4020.013848	-1340.004616	1340.004616	4020.013848	6700.023480
118	-33.00	-6734.897378	-4040.938186	-1346.979395	1346.979395	4040.938186	6734.897378
119	-32.00	-6772.240890	-4063.344292	-1354.448097	1354.448097	4063.344292	6772.240890
120	-31.00	-6811.441797	-4086.864834	-1362.288278	1362.288278	4086.864834	6811.441797
121	-30.00	-6851.835396	-4111.100993	-1370.366998	1370.366998	4111.100993	6851.835396
122	-29.00	-6892.696081	-4135.618602	-1378.539534	1378.539534	4135.618602	6892.696081
123	-28.00	-6933.240289	-4159.943925	-1386.647975	1386.647975	4159.943925	6933.240289
124	-27.00	-6972.598423	-4183.558805	-1394.519602	1394.519602	4183.558805	6972.598423
125	-26.00	-7009.825279	-4205.894917	-1401.964972	1401.964972	4205.894917	7009.825279
126	-25.00	-7043.878423	-4226.326802	-1408.775601	1408.775601	4226.326802	7043.878423
127	-24.00	-7073.605789	-4244.163221	-1414.721074	1414.721074	4244.163221	7073.605789
128	-23.00	-7097.727510	-4258.636252	-1419.545417	1419.545417	4258.636252	7097.727510
129	-22.00	-7114.812619	-4268.887317	-1422.962439	1422.962439	4268.887317	7114.812619
130	-21.00	-7123.248716	-4273.948975	-1424.649658	1424.649658	4273.948975	7123.248716
131	-20.00	-7121.201977	-4272.720931	-1424.240310	1424.240310	4272.720931	7121.201977
132	-19.00	-7106.563957	-4263.938120	-1421.312707	1421.312707	4263.938120	7106.563957
133	-18.00	-7076.880741	-4246.128192	-1415.376064	1415.376064	4246.128192	7076.880741
134	-17.00	-7029.259929	-4217.555706	-1405.851902	1405.851902	4217.555706	7029.259929
135	-16.00	-6960.254374	-4176.152375	-1392.050792	1392.050792	4176.152375	6960.254374
136	-15.00	-6865.737071	-4119.441997	-1373.147332	1373.147332	4119.441997	6865.737071
137	-14.00	-6740.836086	-4044.501410	-1348.167137	1348.167137	4044.501410	6740.836086
138	-13.00	-6580.180644	-3948.108151	-1316.036050	1316.036050	3948.108151	6580.180644
139	-12.00	-6379.331117	-3827.598442	-1275.866147	1275.866147	3827.598442	6379.331117
140	-11.00	-6140.531259	-3684.318536	-1228.106179	1228.106179	3684.318536	6140.531259
141	-10.00	-5895.160745	-3537.096236	-1179.032079	1179.032079	3537.096236	5895.160745
142	-9.00	-5800.120206	-3480.071916	-1160.023972	1160.023972	3480.071916	5800.120206
143	-8.00	-5095.287718	-3057.172449	-1019.057483	1019.057483	3057.172449	5095.287718
144	-7.00	-4338.987448	-2603.392313	-867.797438	867.797438	2603.392313	4338.987448
145	-6.00	-3795.505645	-2277.303251	-759.101084	759.101084	2277.303251	3795.505645
146	-5.00	-3365.781672	-2019.468883	-673.156294	673.156294	2019.468883	3365.781672
147	-4.00	-3002.943994	-1801.766289	-600.588763	600.588763	1801.766289	3002.943994
148	-3.00	-2682.491502	-1609.494805	-536.498268	536.498268	1609.494805	2682.491502
149	-2.00	-2390.548779	-1434.329182	-478.109727	478.109727	1434.329182	2390.548779
150	-1.00	-2118.693758	-1271.216179	-423.738726	423.738726	1271.216179	2118.693758

THE RECIPROCAL TRAP DEPTH

I	E	C=0.0	C=0.2	C=0.4	C=0.6	C=0.8	C=1.0
151	0.00	-1861.481656	-1116.888927	-372.296309	372.296309	1116.888927	1861.481656
152	1.00	-1615.178887	-969.107274	-323.035758	323.035758	969.107274	1615.178887
153	2.00	-1377.079260	-826.247507	-275.415836	275.415836	826.247507	1377.079260
154	3.00	-1145.116631	-687.069937	-229.023312	229.023312	687.069937	1145.116631
155	4.00	-917.635612	-550.581334	-183.527111	183.527111	550.581334	917.635612
156	5.00	-691.249852	-415.549886	-138.649962	138.649962	415.949886	693.249852
157	6.00	-470.750264	-282.450141	-94.150047	94.150047	282.450141	470.750264
158	7.00	-249.042275	-149.425356	-49.808452	49.808452	149.425356	249.042275
159	8.00	-27.099828	-16.259896	-5.419965	5.419965	16.259896	27.099828
160	9.00	196.071548	117.642922	39.214307	-39.214307	-117.642922	-196.071548
161	10.00	421.467989	252.880778	84.293593	-84.293593	-252.880778	-421.467989
162	11.00	650.121406	390.072821	130.024274	-130.024274	-390.072821	-650.121406
163	12.00	883.139277	529.883534	176.627845	-176.627845	-529.883534	-883.139277
164	13.00	1121.756401	673.053801	224.351267	-224.351267	-673.053801	-1121.756401
165	14.00	1367.408275	820.444916	273.481639	-273.481639	-820.444916	-1367.408275
166	15.00	1621.842035	973.105163	324.368388	-324.368388	-973.105163	-1621.842035
167	16.00	1887.293193	1132.375848	377.458616	-377.458616	-1132.375848	-1887.293193
168	17.00	2166.780073	1300.067966	433.355989	-433.355989	-1300.067966	-2166.780073
169	18.00	2464.615882	1478.769441	492.923147	-492.923147	-1478.769441	-2464.615882
170	19.00	2787.339734	1672.403741	557.467914	-557.467914	-1672.403741	-2787.339734
171	20.00	3145.494265	1887.296447	629.098816	-629.098816	-1887.296447	-3145.494265
172	21.00	3557.217252	2134.330224	711.443408	-711.443408	-2134.330224	-3557.217252
173	22.00	4056.010119	2433.605926	811.201975	-811.201975	-2433.605926	-4056.010119
174	23.00	4709.038514	2825.422940	941.807647	-941.807647	-2825.422940	-4709.038514
175	24.00	5665.340160	3399.203893	1133.067964	-1133.067964	-3399.203893	-5665.340160
176	25.00	7304.022105	4382.413002	1460.804334	-1460.804334	-4382.413002	-7304.022105
177	26.00	6794.244572	4076.546500	1358.848833	-1358.848833	-4076.546500	-6794.244572
178	27.00	6713.694699	4028.216579	1342.738860	-1342.738860	-4028.216579	-6713.694699
179	28.00	6889.727889	4133.836487	1377.945496	-1377.945496	-4133.836487	-6889.727889
180	29.00	7143.788044	4286.273111	1428.757704	-1428.757704	-4286.273111	-7143.788044
181	30.00	7415.391596	4449.234692	1483.078231	-1483.078231	-4449.234692	-7415.391596
182	31.00	7683.012733	4609.807365	1536.602455	-1536.602455	-4609.807365	-7683.012733
183	32.00	7939.296768	4763.578977	1587.859659	-1587.859659	-4763.578977	-7939.296768
184	33.00	8182.322976	4909.393493	1636.464498	-1636.464498	-4909.393493	-8182.322976
185	34.00	8412.251021	5047.350312	1682.450104	-1682.450104	-5047.350312	-8412.251021
186	35.00	8630.005041	5178.002716	1726.000905	-1726.000905	-5178.002716	-8630.005041
187	36.00	8836.716491	5302.029579	1767.343193	-1767.343193	-5302.029579	-8836.716491
188	37.00	9033.504571	5420.102420	1806.700807	-1806.700807	-5420.102420	-9033.504571
189	38.00	9221.362565	5532.835209	1844.278403	-1844.278403	-5532.835209	-9221.362565
190	39.00	9401.282824	5640.769358	1880.256453	-1880.256453	-5640.769358	-9401.282824
191	40.00	9573.956016	5744.373267	1914.791089	-1914.791089	-5744.373267	-9573.956016
192	41.00	9740.079533	5844.047372	1948.015791	-1948.015791	-5844.047372	-9740.079533
193	42.00	9900.218489	5940.130739	1980.043580	-1980.043580	-5940.130739	-9900.218489
194	43.00	10054.846528	6032.907557	2010.969186	-2010.969186	-6032.907557	-10054.846528
195	44.00	10204.355416	6122.612885	2040.870962	-2040.870962	-6122.612885	-10204.355416
196	45.00	10349.063112	6209.437497	2069.812499	-2069.812499	-6209.437497	-10349.063112
197	46.00	10489.220354	6293.531837	2097.843946	-2097.843946	-6293.531837	-10489.220354
198	47.00	10625.015897	6375.009158	2125.003053	-2125.003053	-6375.009158	-10625.015897
199	48.00	10756.580580	6453.947964	2151.315988	-2151.315988	-6453.947964	-10756.580580
200	49.00	10883.990369	6530.393832	2176.797944	-2176.797944	-6530.393832	-10883.990369

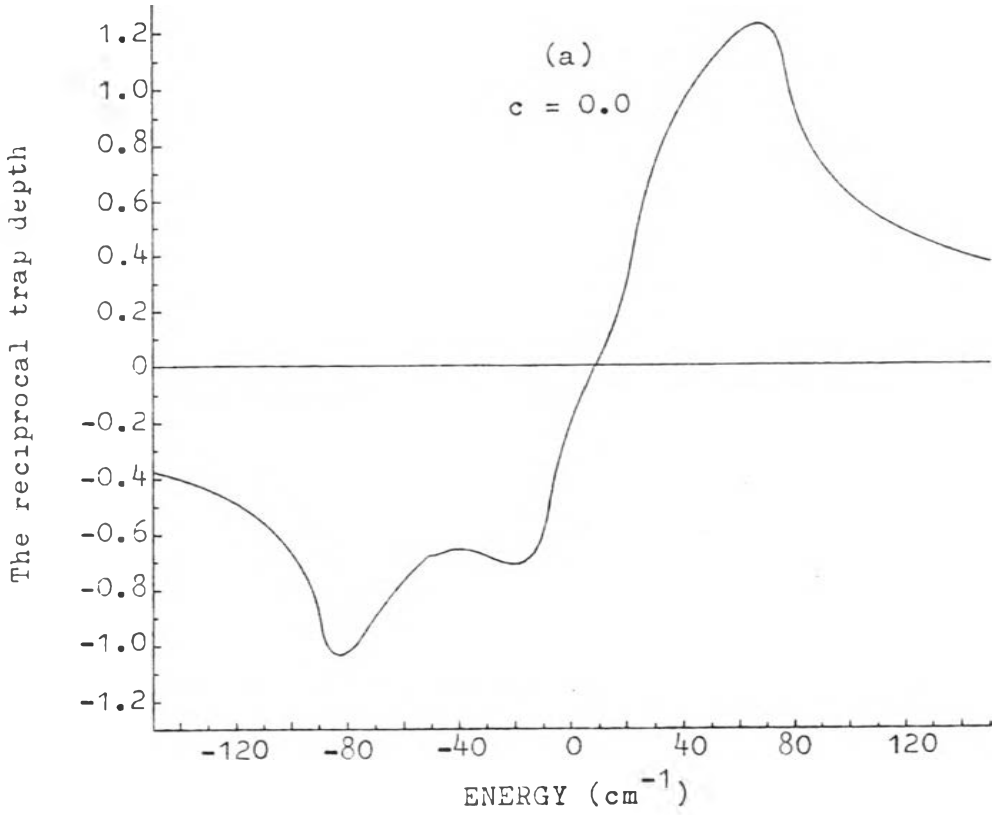
THE RECIPROCAL TRAP DEPTH

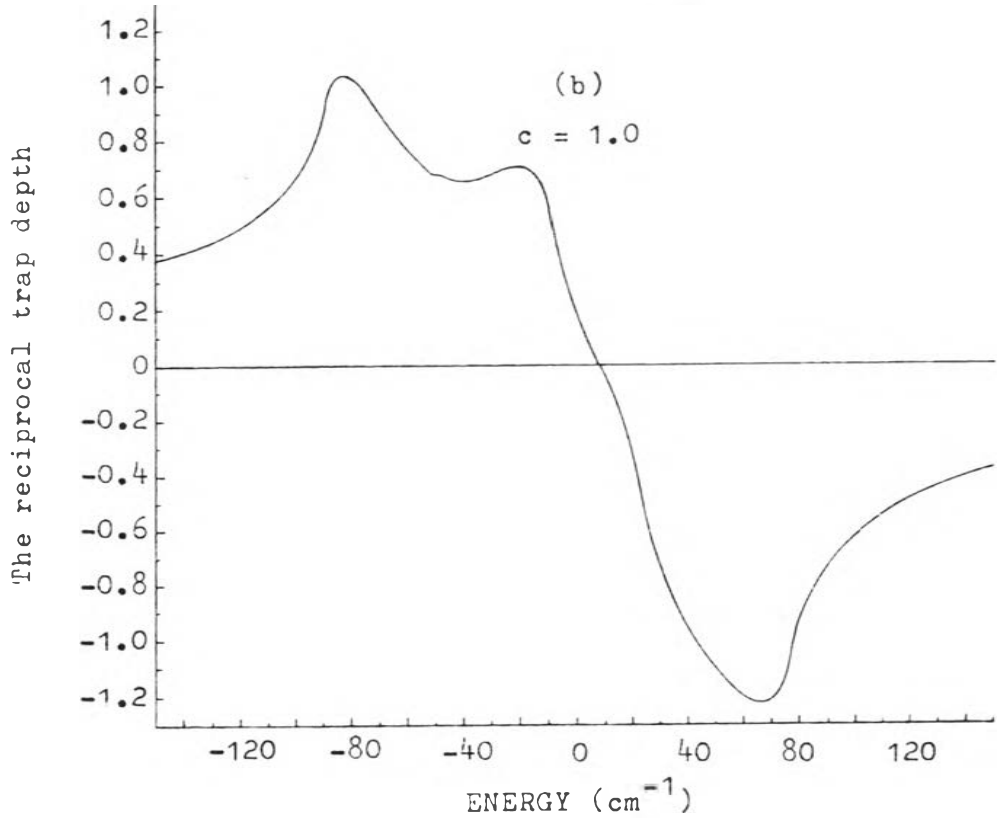
I	E	C=0.0	C=0.2	C=0.4	C=0.6	C=0.8	C=1.0
201	55.00	11307.268498	6604.360705	2201.453568	-2201.453568	-6604.360705	-11007.268498
202	51.00	11126.386825	6675.831697	2225.277232	-2225.277232	-6675.831697	-11126.386825
203	52.00	11241.266451	6744.759469	2248.253156	-2248.253156	-6744.759469	-11241.266451
204	53.00	11351.777647	6811.066182	2270.355394	-2270.355394	-6811.066182	-11351.777647
205	54.00	11457.739095	6874.643048	2291.547683	-2291.547683	-6874.643048	-11457.739095
206	55.00	11558.916428	6935.349443	2311.783143	-2311.783143	-6935.349443	-11558.916428
207	56.00	11655.020002	6993.011584	2331.003861	-2331.003861	-6993.011584	-11655.020002
208	57.00	11745.701829	7047.420677	2349.140226	-2349.140226	-7047.420677	-11745.701829
209	58.00	11830.551516	7098.330487	2366.110162	-2366.110162	-7098.330487	-11830.551516
210	59.00	11909.051027	7145.454191	2381.818064	-2381.818064	-7145.454191	-11909.051027
211	60.00	11980.767973	7188.460355	2396.153452	-2396.153452	-7188.460355	-11980.767973
212	61.00	12044.947045	7226.967796	2408.989265	-2408.989265	-7226.967796	-12044.947045
213	62.00	12100.899020	7260.538980	2420.179660	-2420.179660	-7260.538980	-12100.899020
214	63.00	12147.786526	7288.671481	2429.557160	-2429.557160	-7288.671481	-12147.786526
215	64.00	12184.645363	7310.786782	2436.928927	-2436.928927	-7310.786782	-12184.645363
216	65.00	12210.359622	7326.215337	2442.071779	-2442.071779	-7326.215337	-12210.359622
217	66.00	12223.627881	7334.176292	2444.725431	-2444.725431	-7334.176292	-12223.627881
218	67.00	12222.916284	7333.749133	2444.583111	-2444.583111	-7333.749133	-12222.916284
219	68.00	12206.391818	7323.834655	2441.278218	-2441.278218	-7323.834655	-12206.391818
220	69.00	12171.824842	7303.094470	2434.364823	-2434.364823	-7303.094470	-12171.824842
221	70.00	12116.442446	7269.865034	2423.288345	-2423.288345	-7269.865034	-12116.442446
222	71.00	12036.700598	7222.019928	2407.339976	-2407.339976	-7222.019928	-12036.700598
223	72.00	11927.917178	7156.749880	2385.583293	-2385.583293	-7156.749880	-11927.917178
224	73.00	11783.656849	7070.193688	2356.731229	-2356.731229	-7070.193688	-11783.656849
225	74.00	11594.651714	6956.790614	2318.930205	-2318.930205	-6956.790614	-11594.651714
226	75.00	11346.803726	6808.081830	2269.360610	-2269.360610	-6808.081830	-11346.803726
227	76.00	11017.242629	6610.345184	2203.448395	-2203.448395	-6610.345184	-11017.242629
228	77.00	10565.859207	6339.539146	2113.179715	-2113.179715	-6339.539146	-10565.859207
229	78.00	10012.786847	6007.671750	2002.557250	-2002.557250	-6007.671750	-10012.786847
230	79.00	9574.533980	5744.720146	1914.906682	-1914.906682	-5744.720146	-9574.533980
231	80.00	9218.301449	5530.980539	1843.660180	-1843.660180	-5530.980539	-9218.301449
232	81.00	8915.581750	5349.348731	1783.116244	-1783.116244	-5349.348731	-8915.581750
233	82.00	8650.595729	5190.357128	1730.119043	-1730.119043	-5190.357128	-8650.595729
234	83.00	8413.836185	5048.283410	1682.761137	-1682.761137	-5048.283410	-8413.836185
235	84.00	8199.035553	4919.421039	1639.807013	-1639.807013	-4919.421039	-8199.035553
236	85.00	8002.053456	4801.231788	1600.410596	-1600.410596	-4801.231788	-8002.053456
237	86.00	7819.828529	4691.896838	1563.965613	-1563.965613	-4691.896838	-7819.828529
238	87.00	7650.105966	4590.063306	1530.021102	-1530.021102	-4590.063306	-7650.105966
239	88.00	7491.155848	4494.693241	1498.231080	-1498.231080	-4494.693241	-7491.155848
240	89.00	7341.616195	4404.969454	1468.323151	-1468.323151	-4404.969454	-7341.616195
241	90.00	7200.391134	4320.234423	1440.078141	-1440.078141	-4320.234423	-7200.391134
242	91.00	7066.532534	4239.919268	1413.306423	-1413.306423	-4239.919268	-7066.532534
243	92.00	6939.442660	4163.665360	1387.888453	-1387.888453	-4163.665360	-6939.442660
244	93.00	6818.340637	4091.004139	1363.668046	-1363.668046	-4091.004139	-6818.340637
245	94.00	6702.737782	4021.642430	1340.547477	-1340.547477	-4021.642430	-6702.737782
246	95.00	6592.169605	3955.301527	1318.433842	-1318.433842	-3955.301527	-6592.169605
247	96.00	6486.231941	3891.738933	1297.246311	-1297.246311	-3891.738933	-6486.231941
248	97.00	6384.570362	3830.741989	1276.913996	-1276.913996	-3830.741989	-6384.570362
249	98.00	6286.871891	3772.122910	1257.374303	-1257.374303	-3772.122910	-6286.871891
250	99.00	6192.859428	3715.714835	1238.571612	-1238.571612	-3715.714835	-6192.859428

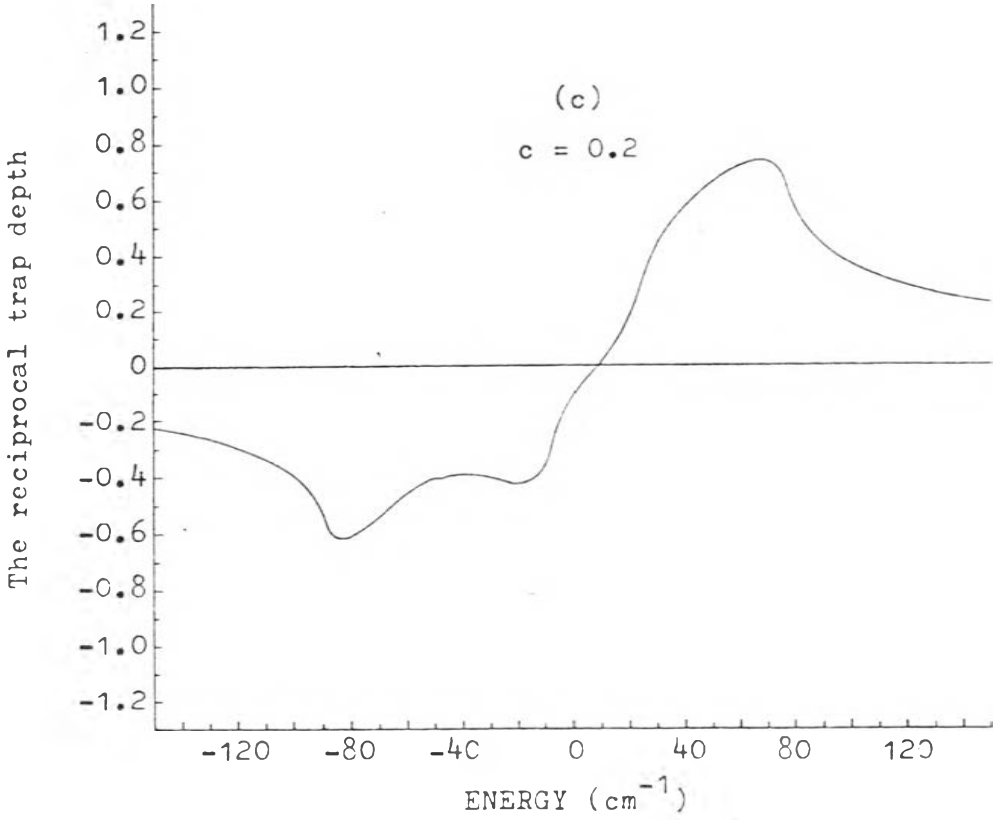
THE RECIPROCAL TRAP DEPTH

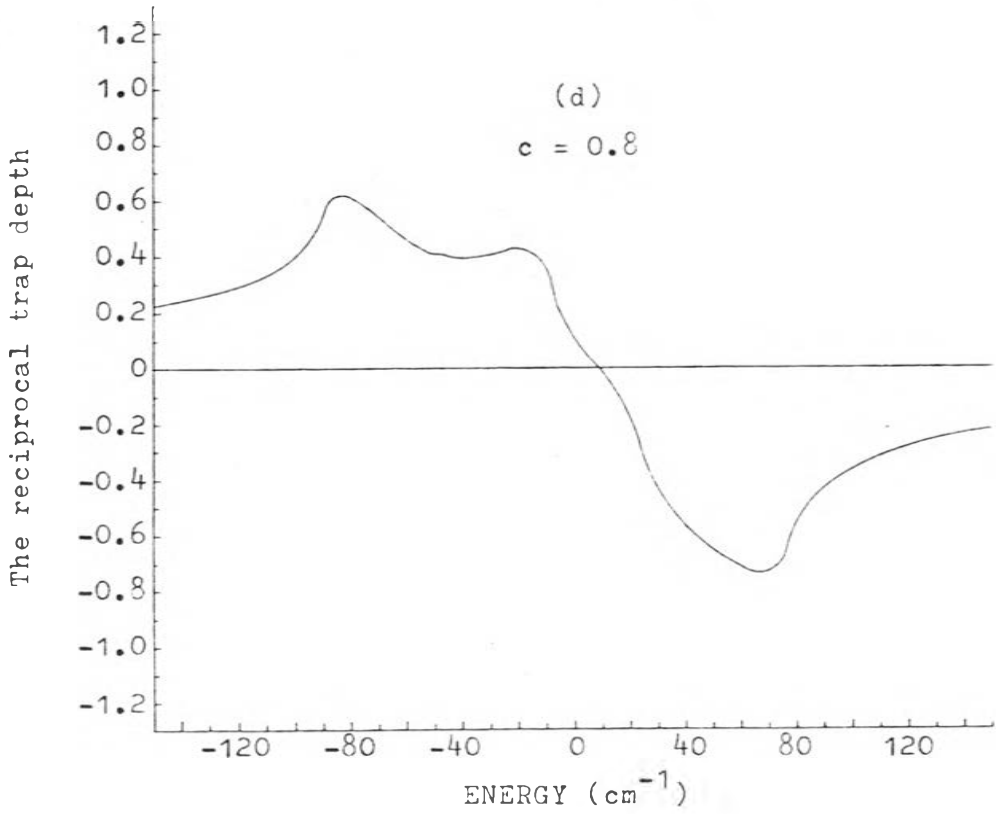
I	E	C=0.0	C=0.2	C=0.4	C=0.6	C=0.8	C=1.0
251	100.00	6102.281488	3661.368874	1220.456225	-1220.456225	-3661.368874	-6102.281488
252	101.00	6014.917926	3608.950541	1202.983514	-1202.983514	-3608.950541	-6014.917926
253	102.00	5930.566441	3558.339652	1186.113217	-1186.113217	-3558.339652	-5930.566441
254	103.00	5849.044678	3509.426598	1169.808866	-1169.808866	-3509.426598	-5849.044678
255	104.00	5770.186823	3462.111888	1154.037296	-1154.037296	-3462.111888	-5770.186823
256	105.00	5693.841571	3416.304739	1138.768246	-1138.768246	-3416.304739	-5693.841571
257	106.00	5619.870418	3371.922050	1123.974017	-1123.974017	-3371.922050	-5619.870418
258	107.00	5548.146197	3328.887520	1109.629173	-1109.629173	-3328.887520	-5548.146197
259	108.00	5478.551831	3287.130903	1095.710301	-1095.710301	-3287.130903	-5478.551831
260	109.00	5410.979259	3246.587362	1082.195787	-1082.195787	-3246.587362	-5410.979259
261	110.00	5345.328497	3207.196907	1069.065636	-1069.065636	-3207.196907	-5345.328497
262	111.00	5281.506833	3168.903911	1056.301304	-1056.301304	-3168.903911	-5281.506833
263	112.00	5219.428118	3131.656684	1043.885561	-1043.885561	-3131.656684	-5219.428118
264	113.00	5159.012140	3095.407099	1031.802366	-1031.802366	-3095.407099	-5159.012140
265	114.00	5100.184082	3060.110267	1020.036756	-1020.036756	-3060.110267	-5100.184082
266	115.00	5042.874033	3025.724240	1008.574747	-1008.574747	-3025.724240	-5042.874033
267	116.00	4987.016563	2992.209759	997.403253	-997.403253	-2992.209759	-4987.016563
268	117.00	4932.550336	2959.530025	986.510008	-986.510008	-2959.530025	-4932.550336
269	118.00	4879.417771	2927.650488	975.883496	-975.883496	-2927.650488	-4879.417771
270	119.00	4827.564736	2896.538869	965.512890	-965.512890	-2896.538869	-4827.564736
271	120.00	4776.940275	2866.163994	955.387998	-955.387998	-2866.163994	-4776.940275
272	121.00	4727.496355	2836.497644	945.499215	-945.499215	-2836.497644	-4727.496355
273	122.00	4679.187653	2807.512424	935.837475	-935.837475	-2807.512424	-4679.187653
274	123.00	4631.971342	2779.182640	926.394213	-926.394213	-2779.182640	-4631.971342
275	124.00	4585.806921	2751.483989	917.161330	-917.161330	-2751.483989	-4585.806921
276	125.00	4540.656037	2724.393460	908.131153	-908.131153	-2724.393460	-4540.656037
277	126.00	4496.482342	2697.889244	899.296415	-899.296415	-2697.889244	-4496.482342
278	127.00	4453.251351	2671.950651	890.650217	-890.650217	-2671.950651	-4453.251351
279	128.00	4410.930316	2646.558032	882.186011	-882.186011	-2646.558032	-4410.930316
280	129.00	4369.488114	2621.692712	873.897571	-873.897571	-2621.692712	-4369.488114
281	130.00	4328.895137	2597.336927	865.778976	-865.778976	-2597.336927	-4328.895137
282	131.00	4289.123195	2573.473764	857.824588	-857.824588	-2573.473764	-4289.123195
283	132.00	4250.145430	2550.087106	850.029035	-850.029035	-2550.087106	-4250.145430
284	133.00	4211.936230	2527.161587	842.387196	-842.387196	-2527.161587	-4211.936230
285	134.00	4174.471154	2504.682543	834.894181	-834.894181	-2504.682543	-4174.471154
286	135.00	4137.726864	2482.635971	827.545324	-827.545324	-2482.635971	-4137.726864
287	136.00	4101.681056	2461.008487	820.336162	-820.336162	-2461.008487	-4101.681056
288	137.00	4066.312401	2439.787295	813.262432	-813.262432	-2439.787295	-4066.312401
289	138.00	4031.600492	2418.960151	806.320050	-806.320050	-2418.960151	-4031.600492
290	139.00	3997.525788	2398.515330	799.505110	-799.505110	-2398.515330	-3997.525788
291	140.00	3964.069570	2378.441600	792.813867	-792.813867	-2378.441600	-3964.069570
292	141.00	3931.213889	2358.728193	786.242731	-786.242731	-2358.728193	-3931.213889
293	142.00	3898.941534	2339.364781	779.788260	-779.788260	-2339.364781	-3898.941534
294	143.00	3867.235984	2320.341452	773.447151	-773.447151	-2320.341452	-3867.235984
295	144.00	3836.081378	2301.648690	767.216230	-767.216230	-2301.648690	-3836.081378
296	145.00	3805.462475	2283.277349	761.092450	-761.092450	-2283.277349	-3805.462475
297	146.00	3775.364628	2265.218642	755.072881	-755.072881	-2265.218642	-3775.364628
298	147.00	3745.773750	2247.464116	749.154705	-749.154705	-2247.464116	-3745.773750
299	148.00	3716.676286	2230.005639	743.335213	-743.335213	-2230.005639	-3716.676286
300	149.00	3688.059192	2212.835383	737.611794	-737.611794	-2212.835383	-3688.059192
301	150.00	3659.909903	2195.945811	731.981937	-731.981937	-2195.945811	-3659.909903

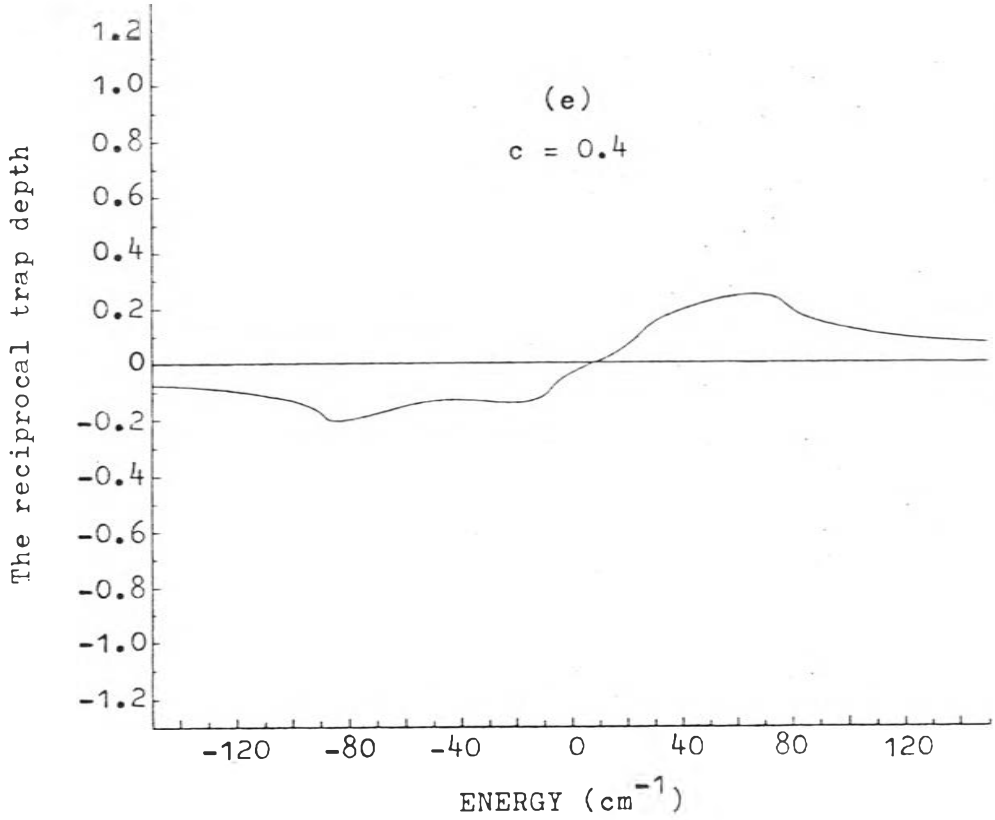
Fig. 4.4.1 Graphical represention of the results listed in Table 4.4.1 [$1/\Delta$ have the dimension $(51.2)^{-1}$ cm in the scales on graphs]

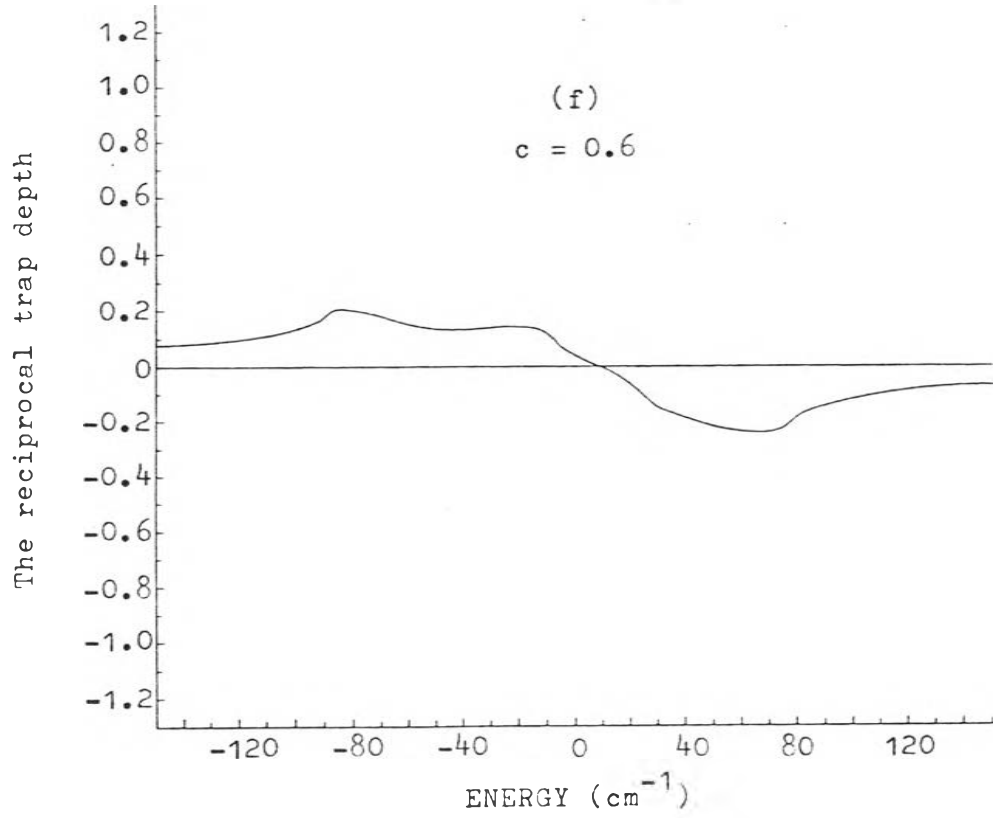

(a)
c = 0.0
The reciprocal trap depth
1.2
1.0
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1.0
-1.2
-120
-80
-40
0
40
80
120
ENERGY (cm^{-1})


(b)
c = 1.0
The reciprocal trap depth
1.2
1.0
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1.0
-1.2
-120
-80
-40
0
40
80
120
ENERGY (cm^{-1})


(c)
c = 0.2
The reciprocal trap depth
1.2
1.0
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1.0
-1.2
-120
-80
-40
0
40
80
120
ENERGY (cm^{-1})


(d)
c = 0.8
The reciprocal trap depth
1.2
1.0
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1.0
-1.2
-120
-80
-40
0
40
80
120
ENERGY (cm^{-1})


(e)
c = 0.4
The reciprocal trap depth
1.2
1.0
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1.0
-1.2
-120
-80
-40
0
40
80
120
ENERGY (cm^{-1})


(f)
c = 0.6
The reciprocal trap depth
1.2
1.0
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1.0
-1.2
-120
-80
-40
0
40
80
120
ENERGY (cm^{-1})