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PROPERTIES AND DISTRIBUTION FUNCTIONS OF POLAR FLUIDS BY PERTURBATION THEORY

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THE UNIVERSITY OF OKLAHOMA

GRADUATE COLLEGE

PROPERTIES AND DISTRIBUTION FUNCTIONS OF POLAR FLUIDS BY PERTURBATION THEORY

A DISSERTATION

SUBMITTED TO THE GRADUATE FACULTY

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degree of

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By

EYNOLLAH ASSAD

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PROPERTIES AND DISTRIBUTION FUNCTIONS OF POLAR FLUIDY BY PERTURBATION THEORY

A DISSERTATION

APPROVED FOR THE

DEPARTMENT OF PHYSICS & ASTRONOMY

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ABSTRACT

It is proposed that perturbation theories and computer simulation be collectively applied to the study of static and dynamic properties of liquids and dense fluids composed of highly nonspherical and/or polar molecules. Perturbation theories rooted in classical statistical mechanics have, in recent years, proven successful in predicting the equilibrium properties of atomic fluids and molecular fluids composed of weakly anisotropic molecules. We propose to develop and test analogous theories for the thermodynamic and transport properties of fluids containing nighly anisotropic molecules. New theories for equilibrium properties will be based on a first order expansion of the angular pair correlation function $g(r\omega_1\omega_2)$, or, equivalently, the function $y(r\omega_1\omega_2)$. Expansions about spherical and nonspherical reference fluids will be explored for static properties. A major strength of the proposed work is the concurrent use of computer simulation to guide and evaluate development of the theories. The investigation includes two different temperatures; $T^*=1.294$ and $T^*=1.277$, with two quadrupole moments of $Q^*=1$ and $Q^*=0.5$, respectively. The density is assumed to be $\rho^*=0.85$.

CHAPTER I

INTRODUCTION

Recently there have been several extensions to the polar system of the theoretical techniques that proved useful in predicting the thermodynamics of simpler fluids. Computational work (1-4) has allowed the evaluation of these theories for uncomplicated models consisting of dipoles embedded in otherwise spherical molecules.

The most surprising success among the theories was a special version of the thermodynamic perturbation theory (5), the so-called Padé approximation due to Stell, Rasaiah and others (6-8). Especially in the last decade there has been great enthusiasm among the laboratory experimentalists, statistical mechanical theorists and those who simulate fluids on the computer because of new developments in the study of the liquid and dense fluid states of matter with the equilibrium properties of "simple" fluids composed of atoms (Ar, Kr) or nearly spherical (CH_4, O_2) molecules.

The most important of these developments was the theoretical development of the perturbation concept which occurred in equilibrium statistical mechanics. This theory is based on the idea that fluids are related to each other and they differ by small amounts of their properties.

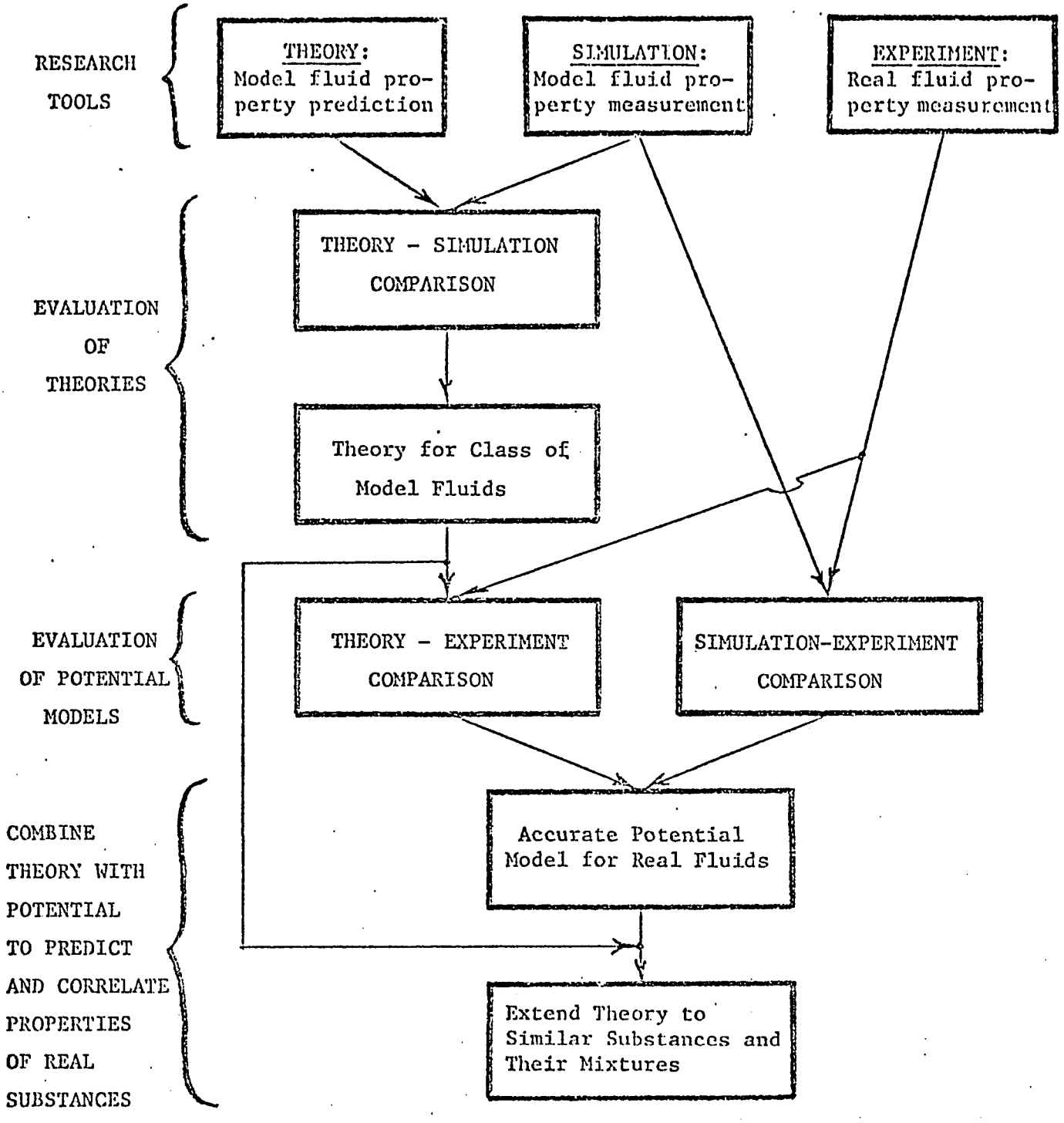
So if we know the properties of a simple fluid, then we can predict the properties of new fluids by treating the differences as perturbed parts. Now this perturbed part has to be calculated successfully. And this "reference" substance can be compared with the results obtained from simulation methods embodied in Monte Carlo and molecular dynamics (9-10) which are available to us.

Figure 1 shows the importance of simulation in providing data for model fluids. Thus, the accuracy of our predictions can be found out by comparing theoretical predictions with simulation results, and by comparing the simulation results with laboratory measurements we can learn about the accuracy of models with real fluids of interest.

The test would be on static properties of the class of model fluids composed of highly nonspherical and/or strongly polar molecules. The reasons can be explained from several viewpoints. From the theoretical point of view, there are presently very few satisfactory theories for predicting the static properties of such fluids. Not very much work has been done on developing perturbation expansions about nonspherical reference fluids which would be applicable to highly anisotropic molecules. There have been a number of thermodynamic perturbation theories developed in the last decade, but most of them are expansions of the Helmholtz free energy or the property of interest directly. But our approach to the equilibrium properties of molecular fluids will be via

second order perturbation theory for the angular pair correlation function $g(r_{12},\omega_1,\omega_2)$. Since the expansion of $g(r_{12},\omega_1,\omega_2)$ is equivalent to the free energy expansion (11) and $g(r_{12},\omega_1,\omega_2)$ can be obtained by computer simulation via a spherical harmonic expansion in the molecular orientations ω_1 and ω_2 (11,13), other equilibrium properties may be obtained from standard formulas in statistical mechanics (14). The success of perturbation theories developed to date has been limited to atomic fluids or to those containing weakly anisotropic molecules for which a spherical reference fluid can be used.

Figure 1: STRATEGY FOR STUDY OF LIQUIDS AND MIXTURES



CHAPTER II

LITERATURE REVIEW

Although the perturbation expansion of the angular pair correlation function $g(r_{12},\omega_1,\omega_2)$ provides an alternate route to macroscopic thermodynamic properties (e.g., free energy, pressure, internal energy) of polar fluids having moderately strong multipolar strengths, expansion of $g(r_{12},\omega_1,\omega_2)$ has received much less attention than the free energy expansion.

Among those theories perhaps one of the best is the Padé extension to third order of the Pople expansion of the free energy due to Stell et al. (14,15); the idea here also is to find the perturbed part of the fluid of interest from the reference system.

$$v(\chi_i,\chi_j) = v_o(r) + \Sigma_\kappa \lambda_\kappa \omega(\chi_i,\chi_j); \qquad \lambda_\kappa \geq 0 \qquad (2\text{-}1)$$

where $v(\chi_i,\chi_j)$ is the orientational part of the pair potential for two molecules and $v_o(r)$ is spherically symmetric reference system), $\{\lambda_\kappa\}$ are related to the dipole moment μ, the quadrupole moment σ, and the octupole moment Φ ..... From recent evidence of computer simulation, the Padé expansion for the free energy in a quadrupole fluid up to moderate values of the quadrupole moment $Q(\varepsilon\sigma^5)^{-\frac{1}{2}}$ of $0(1)$) (16) is promising. The Padé expansion for dipoles contains the correct low and high dipolar strength limits and Padé must be (almost)

correctly interpolating at moderate dipolar strengths, but the Pade' theory breaks down at high anisotropy in anisotropic overlap fluids (17,18).

One of the early expansions of $g(r,\omega_1,\omega_1)$ was done by Gubbins and Gray. They wrote the first order expansion which is valid for a Pople reference and multipolar anisotropics (19).

$$g(r_{12},\omega_1,\omega_2) = g_o(r)(1-EXP(\beta u_a(r,\omega_1,\omega_2))) \qquad (2-2)$$

where $\beta = 1/KT$, u_a the reference fluid radial distribution function. This equation also breaks down for moderately strong anisotropics in that nonphysical, negative values of $g(r_{12},\omega_1,\omega_2)$ are obtained for certain pair orientations.

Perram and White also gave a first order theory of $g(r_{12},\omega_1,\omega_2)$ by using a reference potential of the log-exp mean type on u_a. They only tested the theory for the center pair correlation function $g_c(r)$ (20). Henderson and Gray assumed the potential to consist of two parts: u_a+u_o, where u_a was quadrupole-quadrupole interaction and u_o was a reference potential and then they suggested a perturbation theory involving an expansion of the direct correlation function $C(r,\omega_1,\omega_2)$ (22) in the form of $C_a = C_1 + C_2 + C_3 + ...$ where C_n includes all terms in C_a of order $(u_a)^n$.

They considered two possible closures of the Ornstein-Zernicke equation

$$C_a = -g_o u_a + h_o(h_a - C_a) \qquad (2-3)$$

where

$$h_o = g_o - 1$$

(a mean field and a generalized mean field approximation) to obtain $g_o(r,\omega_1,\omega_2)$ from $C(r,\omega_1,\omega_2)$. Anderson, Weeks and Chandler proposed the "blip function theory" for the calculation of radial distribution function and thermodynamic properties of dense fluids. It is written in a form which yields explicit expressions for both the angular and radial correlation of dense fluids of linear molecules (21).

Steel and Sandler compared this approximation with a variety of correlation functions obtained by numerically solving the extended Percus-Yevick equation for non-spherical molecules. They found that agreement is generally good at high densities, but becomes worse at lower densities because of the omission of the effects of attractive interactions in the blip function theory. Also they extended the blip function formula to $g_c(r)$. In addition, Gubbin et al. (25) and Sung Chandler (26) applied Schofield's temperature expansion for g(r) (27) to the first order and made approximations for higher order correlation functions. Although these theories are largely successful for predicting $g_c(r)$ for moderately strong anisotropy, they are, for the most part, first order theories. Hence, they would not be expected to work for strongly anisotropic fluids. More importantly, knowledge of $g_c(r)$ is not sufficient to enable calculation of all thermodynamic properties.

CHAPTER III

SPHERICAL HARMONIC EXPANSION

If we look at OZ equation

$$h(r_{12},\omega_1,\omega_2) = c(r_{12},\omega_1,\omega_2) + \rho\int dr_3 \langle c(r_1,\omega_1,\omega_3)h(r_{32},\omega_3,\omega_2)\rangle_{\omega_3} \tag{3-1}$$

we record the analysis of (3-1) in spherical harmonics. We restrict considerations to linear molecules so that $\omega=(\theta,\phi)$ denotes the orientation of the symmetry axis. Consider any function $F(r,\omega_1,\omega_2)$ that is invariant under simultaneous rotation of r,ω_1 and ω_2. We first Fourier transform the space variable according to

$$F(\kappa,\omega_1,\omega_2) = \int dr\ \exp(i\kappa r) f(r\ \omega_1\ \omega_2) \tag{3-2}$$

then the rotational invariance implies that $F(r,\omega_1,\omega_2)$ and $F(\kappa,\omega_1,\omega_2)$ can be expanded in spherical harmonics

$$F(r,\omega_1,\omega_2) = \sum_{l_1 l_2 l} F(l_1 l_2 l, r)\Psi l_1 l_2 l(\omega_1,\omega_2\omega_r) \tag{3-3}$$

$$F(k,\omega_1,\omega_2) = \sum_{l_1 l_2 l} F(l_1 l_2 l, k)\Psi l_1 l_2 l(\omega_1,\omega_2,\omega_k) \tag{3-4}$$

where r and k are the magnitudes of $\vec{r}$ and $\vec{k}$ and ω_r. ω_k denotes the orientation of r and k here

$$\Psi l_1 l_2 l(\omega_1\omega_2\omega) = \sum_{m_1 m_2 m} C(l_1 l_2 l, m_1 m_2 m)\cdot Y_{l_1}^{m_1}(\omega_1) Y_{l_2}^{m_2}(\omega_2) Y_l^{m*}(\omega) \tag{3-5}$$

where $Y_l^m(\theta,\phi)$ are spherical harmonics and given by

$$Y_l^m(\omega) = (-1)^m \left(\frac{2l+1}{4\pi}\right)\cdot \frac{(l-m)!}{(l+m)!}\Big)^{\frac{1}{2}} P_l^m (c_o\theta) e^{im\Phi} \qquad (3\text{-}6)$$

and the Legendre polynomial $P_l^m(x)$ is

$$P_l^m(x) = \frac{1}{2^l\, l!}(1-x^2)^{m/2} \frac{d^{m+l}}{dx^{m+l}}(x^2-1)^l$$

here $-l \le m \le l$; $l \ge 0$ (3-7)

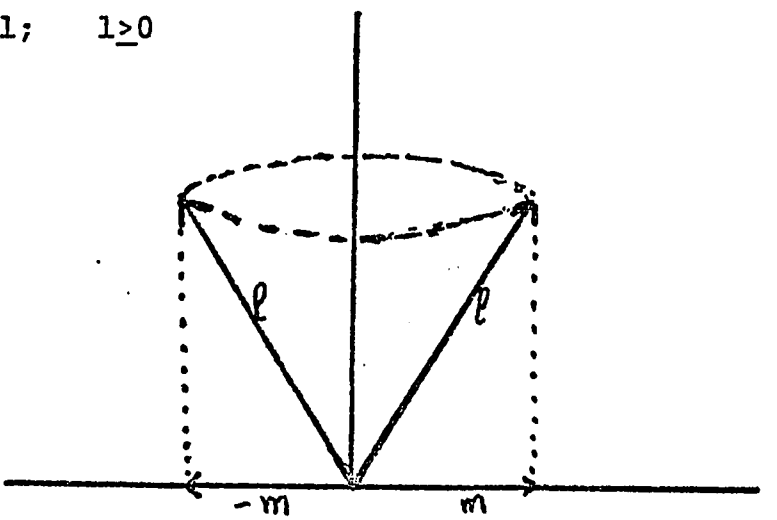


Figure 4

(l is the normal angular moment and m is the azimuthal angular moment), and $C(l_1 l_2 l\ 1, m_1, m_2, m)$ is Clebsch Gordon coefficient. The properties of $C(l_1 l_2 l, m_1 m_2, m)$ are as follows:

$$\sum_l C(l_1 l_2 l, m_1, m-m_1, m) C(l_1 l_2 l', m_1', m'-m_1', m') = \delta_{m_1 m_1'} \delta_{mm'} \qquad (3\text{-}8)$$

$$\sum_m C(l_1 l_2 l, m_1, m-m_1, m) C(l_1 l_2, l', m_1, m-m_1, m) = \delta_{ll'} \qquad (3\text{-}9)$$

and

$$m = m_1 + m \qquad (3\text{-}10)$$

and where δ_{nk} is Kronocker delta function and is

$$\delta_{nk} = \begin{cases} 1 & n=k \\ 0 & n \neq k \end{cases} \qquad (3\text{-}11)$$

Also here $l_1, l_2 l$ must satisfy the triangle relation $\Delta(l_1 l_2 l)$ which we can write as

$$|l_1 - l_2| \leq l \leq (l_1 + l_2) \tag{3-12}$$

Figure 4 shows the l and m. Further, parity considerations for linear molecules shows that $F(l_1, l_2, r) = 0$ unless $l_1 + l_2 + l$ is even. l_1 and l_2 must be drawn from the same set of values, as the symmetry of these functions under interchange of identical molecules implies

$$F(l_1 l_2 l, r) = (-1)^{l_1 + l_2} F(l_2, l_1, l, r) \tag{3-13}$$

CHAPTER IV

SPHERICAL HARMONIC EXPANSION OF THE ANGULAR PAIR CORRELATION FUNCTION

For fluid composed of axially symmetric molecules the angular pair correlation function $g(r,\omega_1,\omega_2)$ can be expanded in terms of product of spherical harmonics of molecular orientation. Rotational invariance of $g(r,\omega_1,\omega_2)$ implies that it depends on only (r,ω_1,ω_2) where $\omega_i = (\Phi_i,\phi_i)$ denotes the orientation of i^{th} molecule with respect to the intermolecular axis.

In this coordinate system, the harmonic series of g is

$$g(r,\omega_1',\omega_2') = 4\pi \sum_{l_1 l_2 m_1} \sum g(l_1 l_2 m_1 r) Y_{l_1}^{m_1}(\omega_1') Y_{l_2}^{\bar{m}_1}(\omega_2') \qquad (4\text{-}1)$$

($\bar{m} = -m$). Only m_i and $\bar{m}_i$ in any terms since the rotational invariance also implies that the ϕ_i can appear only as $\phi_1'-\phi_2'$. Putting the Polar axis in (3-3) in the direction of r so that $\omega_i = \omega_i'$ and subsequently comparing to (4-1) we find

$$g(l_1 l_2 l,r) = 4\pi \left(\frac{4\pi}{2(\ +1)}\right)^{\frac{1}{2}} \sum_{m} C(l_1 l_2 l, m_1 \bar{m}_1 0)\, g(l_1 l_2 m_1, r) \qquad (4\text{-}2)$$

so the desired harmonics in the space fixed axis can be evaluated from knowledge of the body fixed axis $g(l_1 l_2 m_1, r)$. Conversely, the $g(l_1 l_2\ m, r)$ may be found from the $g(l_1 l_2 l, r)$ by

$$g(l_1 l_2 m r_{12}) = (4\pi)^{-3/2} \Sigma_l (2\ +1)^{1/2} g(l_1 l_2 l, r_{12}) C(l_1 l_2 l, m_1 \bar{m}_1 0) \qquad (4\text{-}3)$$

For homonuclear diatomic $(0^2,N^2)$ l_1 and l_2 are both even. The validity of equations (4-3) and (4-2) can be proven by using equation (4-1) and substituting (4-2). In (4-3), we get

$$g(l_1l_2m_1r) = \sum_l \left(\frac{2l+1}{4\pi}\right)^{\frac{1}{2}} C(l_1l_2l, m_1\bar{m}_1o) \left(\frac{4\pi}{2l+1}\right)^{\frac{1}{2}} \left[\sum_m C(l_1l_2lm\ \bar{m}) \cdot (g(l_1l_2mr)\right] = \sum_l \sum_m C(l_1l_2l, m_1\bar{m}_1o) C(l_1l_2l, m\ \bar{m}\ o)$$

$$g(l_1l_2mr) = \sum_m g(l_1l_2mr)_1 C(l_1l_2\ m_1\bar{m}_1o) \cdot C(l_1l_2l, m\ \bar{m}\ o)$$

$$= \sum_m g(l_1l_2m\ r)\,\delta_{mm_1} \qquad (4\text{-}4)$$

With the help of orthogonality condition of spherical harmonic functions, equation (4-1) can be inverted to

$$g(l_1l_2mr) = 4\pi \int d\omega_1' d\omega_2' Y_{l_1}^{m_1*}(\omega_2)\, g(r\omega_1'\omega_2') \qquad (4\text{-}5)$$

This integral can be evaluated by Monte Carlo techniques by taking an average of $Y_{l_1}^{m_1*}(\omega_1')\, Y_{l_2}^{\bar{m},*}(\omega_2)$ over the shell between r and r+Δr in particular

$$g(l_1l_2m_1r) = 4\pi g_{ooo}(r) \langle Y_{l_1}^{m_1}(\omega_1)\, Y_{l_2}^{\bar{m}_1}(\omega_2) \rangle$$

where g_{ooo} is the center pair correlation function g_c and $\langle \ldots\ldots \rangle$ represents an ensemble average over a spherical shell of radius r and thickness Δr. Several workers have used this approach in evaluating $g(r,\omega_1,\omega_2)$ in order to study local structure in fluids composed of linear molecules (6,7,32,33).

Typically, about thirty $g(l_1 l_2 m,r)$ coefficients are evaluated and used to approximate the infinite series of equation (4-1). Convergence of the series appears to be satisfactory for this number of terms.

Figure 2 shows the $g(l_1 l_2 m,r)$ coefficient obtained from a molecular dynamics simulation of a Lennard-Jones plus quadrupole fluid. Figure 3 shows a three dimensional surface of the $g(r,\omega_1,\omega_2)$ function obtained by recombining the expansion of equation (4-1) with the molecular dynamics determined $g(l_1 l_2 m\ r)$. In particular, Figure 3 demonstrates that the quadrupolar anisotropy forces molecular pairs into the "tee" orientation rather than parallel or related orientations in the shell of nearest neighbors.

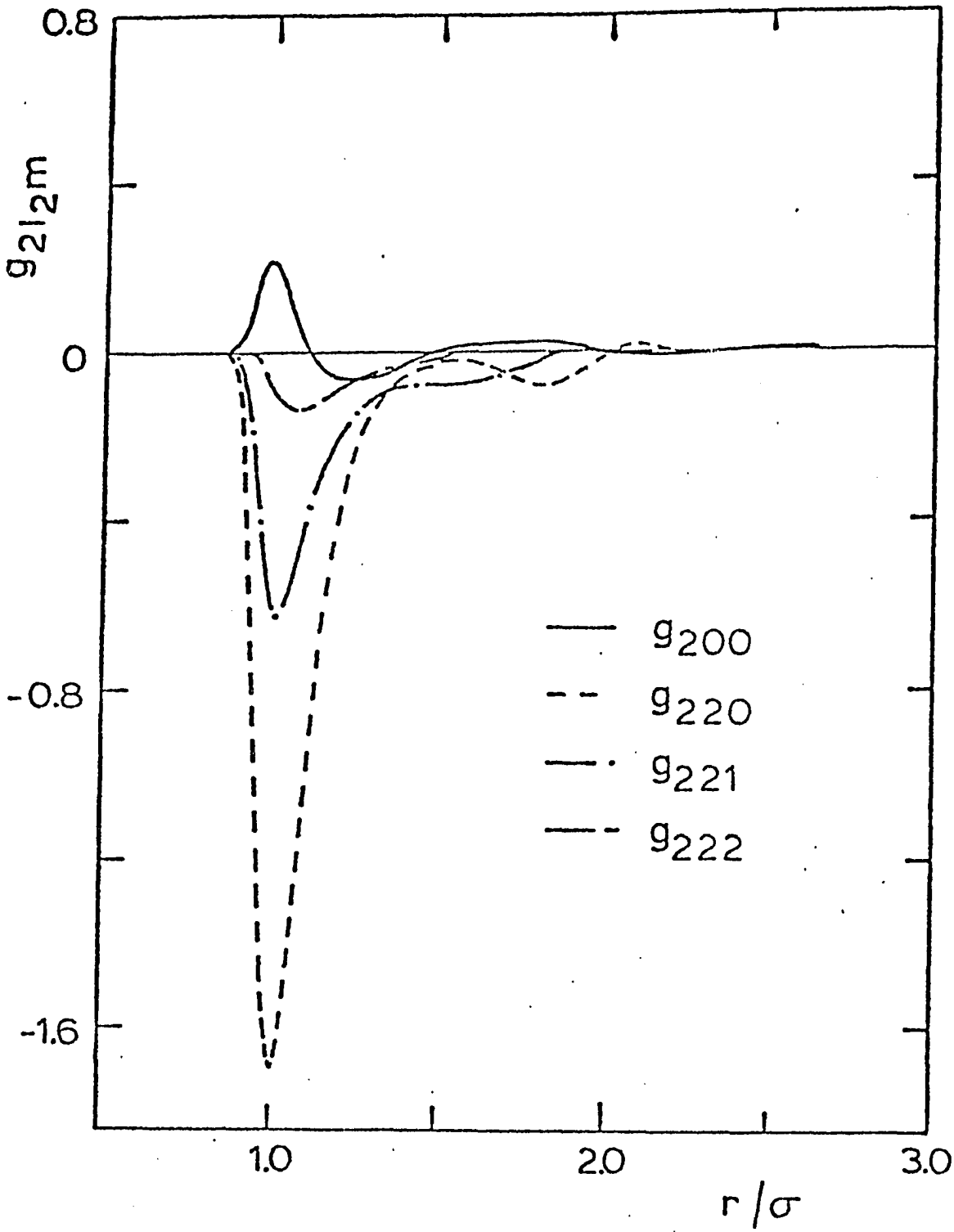


Figure 2 : The $g_{2\ell_2 m}$ coefficients in the Spherical Harmonic Expansion for the Angular Pair Correlation Function for a Lennard-Jones plus Quadrupole Fluid. $KT\varepsilon^{-1} = 1.277$, $\rho\sigma^3 = .85$, $Q(\varepsilon\sigma^5)^{-\frac{1}{2}} = 1$. [2]

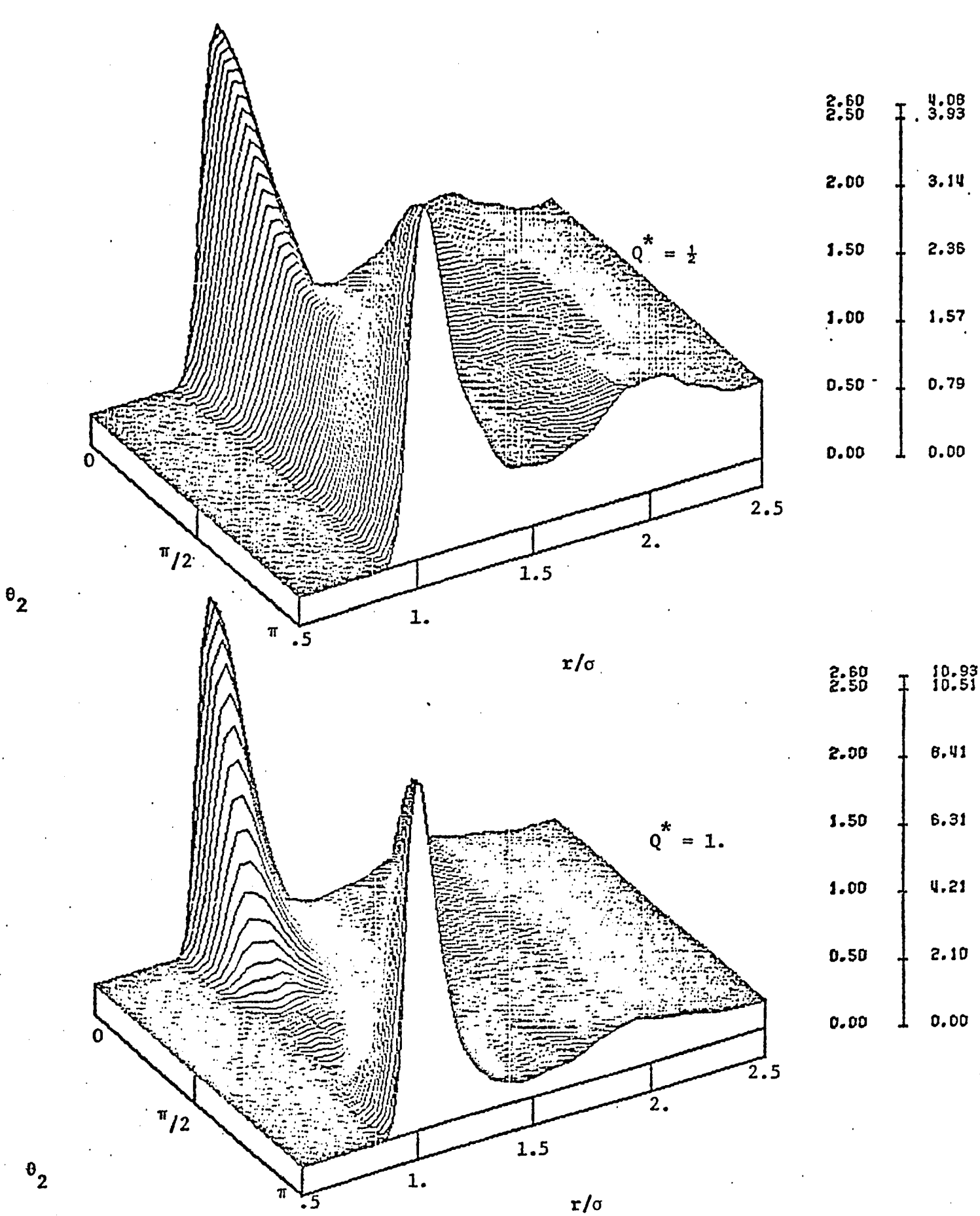


Figure 3 : Effect of the Quadrupole Moment on a Subspace of the Angular Pair Correlation Function for the fluid of Figure 1. Here $\theta_1 = 90$, ϕ undefined [7].

CHAPTER V

THEORY

Our basic approach is derived from the functional derivation formalism of Percus (126) and Lebowitz (124,125) for inhomogeneous systems. In this approach, the inhomogeneity arises due to the "turning on" of an external potential U(r). With proper selection of the generating function, the Percus-Yevick (PY), Hypernetted Chain (HNC) and Yvon-Born-Green (YGB) internal equations were shown to be first order functional Taylor expansions in terms of the singlet density n_1. We first introduce the definitions of the important quantities. The partition function of the inhomogeneous system in a grand canonical ensemble is

$$\Xi(u)=\Sigma_{n\geq 0}(N!_1)^{-1}Z^n\int d\{n\}\exp\{-\beta V_n(\{n\})-\beta\Sigma_i u(i)\} \qquad (5\text{-}1)$$

the singlet density $n_1(1/u)$ is

$$n_1(\frac{1}{u})\equiv\Sigma_{n\geq 1}\frac{Z^n}{(n-1)!}\int d\{n-1\}\exp\{-\beta V_n(\{n\})-\beta\Sigma_i u(i)\} \qquad (5\text{-}2)$$

Here {n} is the set of molecular configurations, {1,2,3,4,.... ....N}, each number i represents the position r_i of the center of mass (com) and orientation (Euler angles)

ω_i of the i^{th} molecule, β is reciprocal temperature $(KT)^{-1}$, K is the Boltzmann constant, Z being the activity

$\exp(\beta\mu)/\lambda^3$, μ the chemical potential, λ the deBroglie thermal wave length, V_N the N body potential assumed to be pair-wise additive.

$$V\{N\} = \sum_i^N \sum_j u(i,j) \tag{5-3}$$

where u is the full pair potential, which is separated into a reference potential U_o and a perturbation term u_p

$$u(12) = u_o(12) + u_p(12) \tag{5-4}$$

where $(12) = (r_{12}, \omega_1, \omega_2)$.

We will talk about the potential in a separate section. To derive the perturbation equation in general, we adopt the generating functional of the PY type, i.e., $\eta_1(\frac{1}{u})\exp(\beta u(1))$. We note that from functional calculus, on Ξ we have the following relations

$$\frac{\partial \ell n \Xi(u)}{\partial \exp -\beta u(1)} = (\exp(\beta u(1)))\eta_1(\frac{1}{u}) \tag{5-5}$$

$$\frac{\partial^2 \ell_n \Xi(u)}{\partial \exp -\beta u(1) \partial \exp -\beta u(2)} = \exp(\beta u(1))\exp(\beta u(2)) \cdot \tag{5-6}$$

$$[\eta_2(\frac{12}{u}) - \eta_1(\frac{1}{u})\eta_1(\frac{2}{u})]$$

$$\frac{\partial^3 \ell_n \Xi(u)}{\partial \exp -\beta u(1) \partial \exp(-\beta u(2)) \partial \exp(-\beta u(3))} = \exp \beta u(1) \exp \beta u(2) \cdot$$

$$\exp \beta u(3) \left[\eta_3(\frac{123}{u}) - \eta_2(\frac{12}{u}) - \eta_1(\frac{3}{u}) - \eta_2(\frac{23}{u})\eta_1(\frac{1}{u})\right.$$

$$\left. -\eta_2(\frac{13}{u})\eta_1(\frac{2}{u}) + 2\eta_1(\frac{1}{u})\eta_1(\frac{2}{u})\eta_1(\frac{3}{u})\right] \tag{5-7}$$

Consider $\eta_1 \exp(\beta u)$ as a functional of $\exp(-\beta u)$ where η_1 is the singlet density and expand to the second order in a functional Taylor series.

$$\eta_1\left(\frac{1}{u}\right) e^{\beta u^o(1)} = \eta_1{}^o\left(\frac{1}{u}\right) e^{\beta u^o(1)} + \int d_3 e^{\beta u^o(1)} e^{\beta u^o(3)} \left[\eta_2\left(\frac{13}{u^o}\right)\right.$$

$$\left. - \eta_1\left(\frac{1}{u^o}\right) \eta_1\left(\frac{3}{u^o}\right)\right] \left[e^{-\beta u(3)} - e^{-\beta u^o(3)}\right] + \frac{1}{2} \int d3d4\ e^{\beta u^o(1)} \cdot$$

$$e^{\beta u^o(3)} e^{\beta u^o(4)} \left[\eta_3\left(\frac{134}{u^o}\right) - \eta_2\left(\frac{13}{u^o}\right) \eta_1\left(\frac{4}{u^o}\right) + 2\eta_1\left(\frac{1}{u^o}\right) \cdot\right.$$

$$\left. \eta_1\left(\frac{3}{u^o}\right) \eta_1\left(\frac{4}{u^o}\right) - \eta_2\left(\frac{14}{u^o}\right) \eta_1\left(\frac{3}{u^o}\right) - \eta_2\left(\frac{34}{u^o}\right) \eta_1\left(\frac{1}{u^o}\right)\right] \cdot$$

$$\left[e^{-\beta u(3)} - e^{-\beta u^o(3)}\right] \left[e^{-\beta u(4)} - e^{-\beta u^o(4)}\right] \qquad (5\text{-}8)$$

This can be reduced to

$$Y(12) = Y^o(12)\ \{1 + \rho \int d3\ \left[\frac{g_3^o(132)}{g^o(12)} - g^o(32)\right] \left[e^{-\beta u(32)} - 1\right] \qquad (5\text{-}9)$$

$$+ \left(\tfrac{1}{2}\right)\ \rho^2 \int d3d4 \left[\frac{g_4^o(1342)}{g^o(12)} - g_3^o(342) - \frac{g_3^o(132) g^o(42)}{g^o(12)}\right.$$

$$\left. - \frac{g_3^o(142) g^o(32)}{g^o(12)} + 2g^o(32) g^o(42)\right] \left[e^{-\beta u(32)} - 1\right]$$

where we have introduced the Y-distribution function $Y(12)$ $g(12)\exp\beta u(12)$. The superscript o represents the reference potential u_o.

To make efficient numerical calculation, the higher order correlation functions g_3, g_4 must be approximated by the two body expressions. The Kirkwood superposition has been intensively used

$$g_3(123) = g(12)g(13)$$

$$g_4(1234) = g_3(123)g_3(134)g_3(124)g_3(234)/(g(12)$$

$$g(13)g(14)g(23)g(24)g(34)) \qquad (5\text{-}11)$$

Jackson and Feenberg (131) gave a "convolution approximation"

$$g_3^{(c)}(123) = 1 + h(12) + h(12)h(23) + \rho\int d4h(14)h(24)h(34)$$

$$+ h(23) + h(23)h(31) + h(31) + h(3)h(12) \qquad (5\text{-}11)$$

For convenience, we develop the perturbation equation with Kirkwood approximation and to the first order terms only.

A similar procedure can be used for the convolution approximation and to the second order terms, substituting the $Y(123)=Y(12)Y(23)Y(13)$ into

$$Y(12) = Y^{o}(12)\{1 + \rho\int d3 \ldots\ldots\ldots\ldots \qquad (5\text{-}12)$$

By keeping only the first order perturbation, we have

$$Y(12) = Y^{o}(12)\{ 1 + \rho^{\Omega-1}\int d3h(13)g^{o}(32)f(32) \qquad (5\text{-}13)$$

where $f(32) = \exp(-\beta u_p(32))-1.$ (5-14)

Ω is the angle normalization constant, e.g., $\Omega=8\pi^2$ for the complete Euler angles of linear molecules.

Figure 5 depicts the geometric arrangement of molecules 1, 2, and 3 for a fluid. We have translational invariance; the change of origin to r_i gives Figure 5.2.

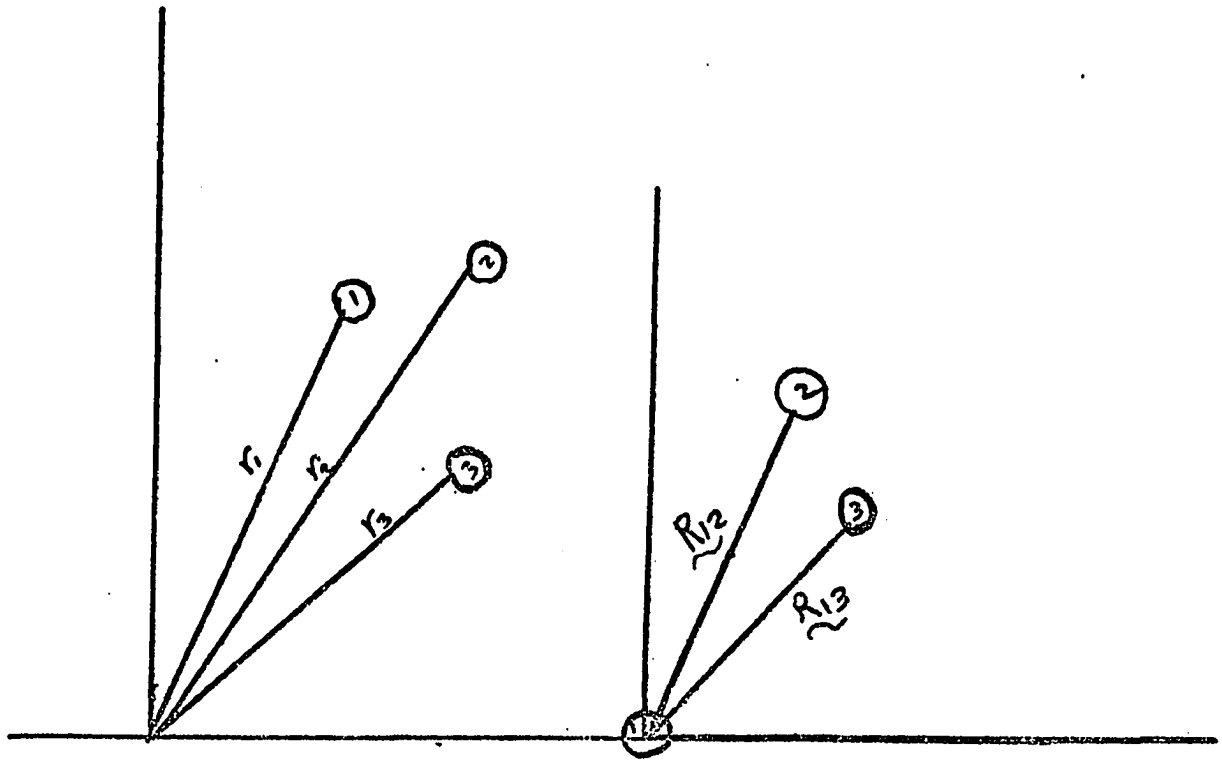


Figure 5.1 Figure 5.2

Equation (5-13) now can be written

$$Y(R_{12}\omega_1\omega_2)=Y^{o}(R_{12}\omega_1\omega_2)\ \{1+\rho\int dR_{13}\langle h(R_{13}\omega_1\omega_3)g^{o}(R_{32}\omega_3\omega_2)$$

$$f(R_{13}\ \omega_3\ \omega_2>\omega_3\} \qquad (5\text{-}15)$$

where $\langle\ldots\ldots\rangle$ is the angle average over ω_3. To evaluate this equation, we expand the three functions Y/Y_0, h and $g^{o}F$ into spherical harmonics

$$\frac{Y(R_{12}\omega_1\omega_2)}{Y_0(R_{12})} = \sum_{\substack{\bar{l}_1\\ \bar{l}\\ \bar{l}}}\ \sum_{\substack{\bar{m}_1\\ \bar{m}_2\\ \bar{m}}}\ \sum_{\substack{\bar{n}_1\\ \bar{n}_2}} E_Y(\bar{l}_1\bar{l}_2\bar{l}\ \bar{n}_1\bar{n}_2R_{12})C(\bar{l}_1\bar{l}_2\bar{l}\ \bar{m}_1\bar{m}_2\bar{m})\cdot$$

$$D^{l_1}_{m_1n_1}{}^{*}(\omega_1)D^{l_2}_{m_2m_2}{}^{*}(\omega_2)Y^{m}_{l}{}^{*}(\Omega_{12}) \qquad (5\text{-}16)$$

$$h(R_{13}\,{}_1\omega_3) = \sum_{\substack{l_1\ m_1\ n_1\\ l_3\ m_3\ n_3\\ l\ m}} E_Y(l_1 l_3 l, n_1 n_3 R_{13}) C(l_1 l_3 l, m_1 m_3 m)$$

$$D^{l_1}_{m_1 n_1}{}^*(\omega_1) D^{l_3}_{m_3 n_3}{}^*(\omega_3) Y^m_l{}^*(\Omega_{13}) \qquad (5\text{-}17)$$

$$g^o(R_{23}\omega_2\omega_3) f(R_{23}\omega_2\omega_3) = \sum_{\substack{l_1\ m_3\ n_3\\ l_2'\ m_2'\ n_2'\\ l'\ m}} E_f(l_3' l_2' l', n_3' n_2' R_{32})$$

$$C(l_3' l_2' l', m_2' m_3' m') D^{l_3'}_{m_3' n_3'}{}^*(\omega_3) D^{l_2'}_{m_2' n_2'}(\omega_2) Y^m_l\ (\Omega_{32}) \qquad (5\text{-}18)$$

Here E are the coefficients of expansion, $C(l_1 l_2 l m_1 m_2 m)$ the Clebsch-Gordon coefficients, D the rotational matrices (see Rose, M. E. "Elementary Theory of Angular Momentum", John Wiley, N.Y., 1957) and Y^m_l the spherical harmonic function.

CHAPTER VI

PROPERTIES OF SPHERICAL HARMONIC COEFFICIENTS

Spherical harmonic coefficients $g(l_1 l_2 lr)$ not only give structural information via equation (4-1) but also are related to numerous equilibrium fluid properties via standard formulae in statistical mechanics (8). Thus, we derive the configurational internal energy in terms of the $g(l_1 l_2 l,r)$ coefficients (17).

A number of these results are summarized in Table 1. In general, the relation in Table 1 involves infinite sums over the indices. However, in the special case of fluids which interact with a Lennard-Jones plus a multipotential, the relations reduce to sum over finite number of terms. For example, Table 2 gives the thermodynamic properties which are the specific equations for the properties of Table 1 for the Lennard-Jones plus quadrupole fluids.

In Table 2 the term $J_n^{l_1 l_2 m}$ represents one dimensional integral over the coefficients $g(l_1 l_2 l,r)$.

$$J_n^{l_1 l_2 m} = \int_o^\infty dr\ r^{-(n-2)} g(l_1 l_2 m,r) \qquad (6\text{-}1)$$

The results in Table 2 have been tested by computer simulation and found to give highly satisfactory agreement (7,17).

TABLE 1

Examples of Expressions for Equilibrium Properties in Terms of Coefficients $u_{\ell_1\ell_2 m}(r)$ and $g_{\ell_1\ell_2 m}(r)$ for Spherical Harmonic Expansions of the Intermolecular Potential $u(r\omega_1\omega_2)$ and Angular Pair Correlation Function $g(r\omega_1\omega_2)$

Configurational Internal Energy

$$U^c/N = \tfrac{1}{2}\rho \sum_{\ell_1\ell_2 m} \int d\underline{r}\; u_{\ell_1\ell_2 m}(r)\; g_{\ell_1\ell_2 m}(r)$$

Pressure

$$P(\rho kT)^{-1} = 1 - \rho\,(6kT)^{-1} \sum_{\ell_1\ell_2 m} \int d\underline{r}\; r\, \frac{du_{\ell_1\ell_2 m}(r)}{dr}\, g_{\ell_1\ell_2 m}(r)$$

Isothermal Compressibility

$$\chi = (\rho kT)^{-1} + (kT)^{-1} \int d\underline{r}\; (g_{ooo}(r) - 1)$$

Mean Squared Torque

$$\langle \tau^2 \rangle = -\rho kT \sum_{\ell_1\ell_2 m} \ell_1(\ell_1+1) \int d\underline{r}\; g_{\ell_1\ell_2 m}(r)\; u_{\ell_1\ell_2 m}(r)$$

Kirkwood Angular Correlation Parameters

$$G_L = (2L+1)^{-1} \rho \sum_m (-1)^m \int d\underline{r}\; g_{LLm}(r)$$

G_o, G_1, G_2 are related to the isothermal compressibility, dielectric constant, and Kerr constant, respectively.

TABLE 2

Examples of Expressions for Equilibrium Properties of a Lennard-Jones plus Quadrupole Fluid in Terms of the $J_n^{\ell_1\ell_2 m}$ Integrals of Equation (4)

Configurational Internal Energy

$$U^c/N = 8\pi\rho^*\epsilon[J_{12}^{\ 000} - J_6^{\ 000}] + U_{QQ}$$

$$U_{QQ} = \frac{12\pi}{5}\rho^* Q^{*2}\epsilon[J_5^{\ 220} + \frac{4}{3}J_5^{\ 221} + \frac{1}{3}J_5^{\ 222}]$$

where $\rho^* = \rho\sigma^3$ and $Q^* = Q(\epsilon\sigma^5)^{-\frac{1}{2}}$

Pressure

$$P(\rho kT)^{-1} = 1 - 16\pi\rho^*(kT)^{-1}[J_6^{\ 000} - 2J_{12}^{\ 000}] - \frac{5}{3}(kT)^{-1}U_{QQ}$$

Mean Squared Torque

$$\langle\tau^2\rangle = -12\epsilon T\, U_{QQ}$$

Kirkwood Angular Correlation Functions

$$G_L = \frac{4\pi\rho^*}{2L+1}\sum_m (-1)^m J_o^{\ LLm}$$

CHAPTER VII

POTENTIAL MODELS

Recently a new approach to the potential model has been developed. The potentials consist of two parts: $u=u_o+u_a$. The reference system is one in which the molecules interact with an isotropic pair potential $u_o(R_{12})$ defined by

$$u_o(R_{12}) = \langle u(R_{12}\omega_1\omega_1)\rangle_{\omega_1\omega_2} \tag{7-1}$$

where $u(R_{12},\omega_1,\omega_2)$ is the pair potential for the actual system.

This pair potential is $U(R_{12}\omega_1\omega_2) = U(R_{12},\theta_1,\theta_2,\phi_{12})$ and the one which has been chosen for study here

$$u(R_{12},\theta_1,\theta,\phi_{12}) = 4\varepsilon[(\frac{\sigma}{R_{12}})^{12} - (\frac{\sigma}{R_{12}})^{6}] + u_a \tag{7-2}$$

with the angle dependent part of the potential defined so that $\langle u_{a\omega_i\omega_2}\rangle = 0$; thus for equation (7-1), u_o is the Lennard-Jones (12,6) potential. In general, there are several choices for u_a available. The choice depends on the system being investigated. These several parts are:

(1) Dipole-dipole part

$$u_{DD}(12) = -\frac{\mu^2}{R_{12}^2}[2C_1C_2 - S_1S_2C_{12}] \tag{7-3}$$

(2) Dipole-quadrupole part

$$u_{DQ}(12) = \left(\frac{3}{2}\frac{Q\,\mu}{R_{12}^4}\right)[C_1(3C_2^2-1) - C_2(3C_1^2-1) - 2(C_2 - C_1)\cdot S_1S_2C_{12}] \quad (7\text{-}4)$$

(3) Quadrupole-quadrupole interaction

$$u_{QQ}(12) = \left(\frac{3}{4}\frac{Q^2}{R_{12}^5}\right)[1 - 5C_1^2 - 5C_2^2 - 15C_1^2C_2^2 + 2(S_1S_2C_{12} - 4C_1C_2)^2] \quad (7\text{-}5)$$

(4) Anisotropic overlap interaction

$$u_a = 4E\left(\frac{\delta}{R_{12}}\right)^{12}(3C_1^2 + 3C_2^2 - 2) \quad (7\text{-}6)$$

In these equations, $S_1 = \sin\theta_i$, $C_1 = \cos\theta$, $C_{12} = \cos(\phi_1 - \phi_2)$ so $C_{12} = \cos\phi_{12}$. u and Q are dipole and quadrupole moments, respectively, and δ is a dimensionless overlap constant $(-0.25<\delta<0.5)$, θ_1, θ_2, ϕ_{12} are the usual orientation angles, referred to the line between molecular centers as polar axis. Figure 7.1 shows the orientation angles in the body fixed coordinate.

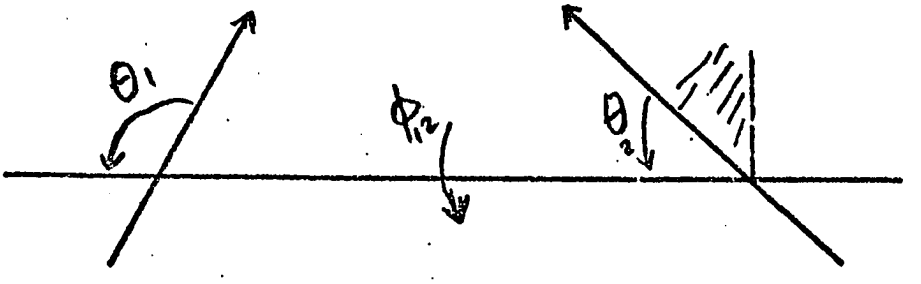
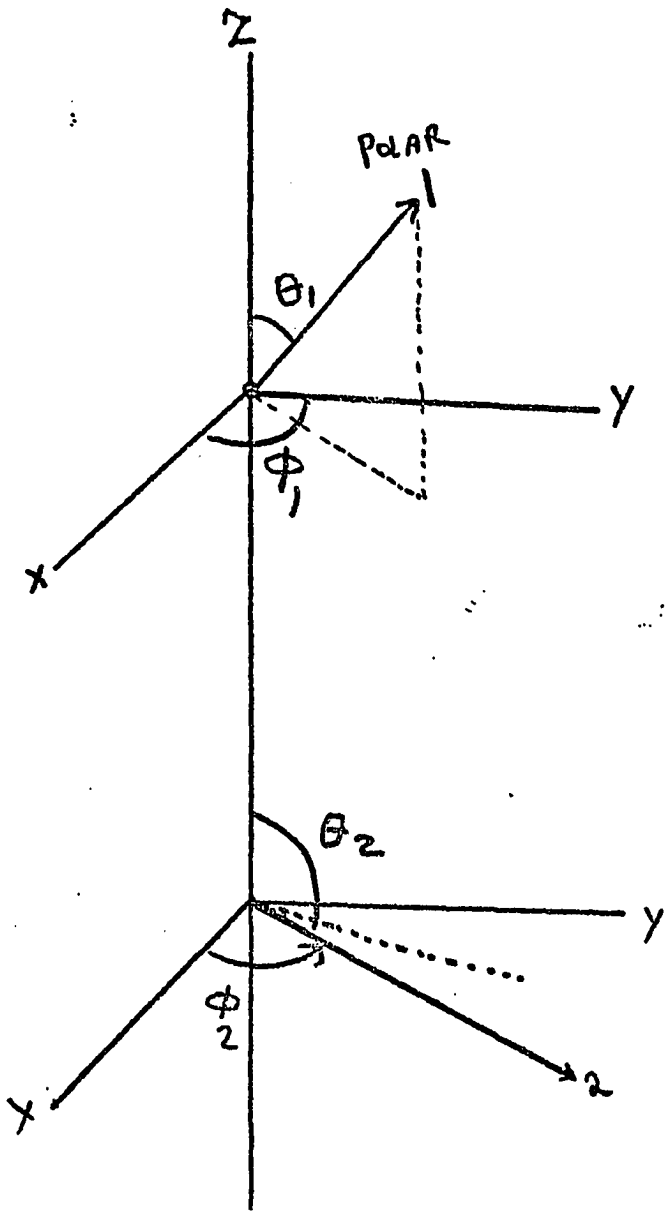


Figure 7.1: The Orientation Angles in the Body Fixed Coordinate

Potential Model



θ_1, ϕ_1

θ_2, ϕ_2

$\phi_{12} = \phi_1 - \phi_2$

Figure 7.2

In our study, the perturbing potential part is the (quadrupole-quadrupole) interaction in the body fixed coordinate. We can expand this potential as

$$u_{QQ}(12) = 4\pi \sum_{m=-2}^{2} (-1)^{(2+m)} X^{22m}\, Y_2^m(\omega_1) Y_2^{m*}(\omega_2) \qquad (7\text{-}7)$$

where

$$X^{22-2} = X^{222} = \frac{1}{6} \cdot \frac{6}{5} \frac{Q^2}{R^5} = \frac{1}{5} \frac{Q^2}{R^5}$$

$$X^{22-1} = X^{221} = \frac{2}{3} X^{220}$$

$$X^{220} = \frac{6}{5} \frac{Q^2}{R^5} \qquad (7\text{-}8)$$

And in the space fixed coordinate, we can expand

$$u_{QQ}(12) = \sum_{l} \sum_{m_1=-2}^{2} \sum_{m_2=-2}^{2} f(221,R) C(221, m_1 m_2 m) Y_2^{m_1}(\omega_1) Y_2^{m_2}(\omega_2) \cdot$$

$$Y_l^m(\Omega) \qquad (7\text{-}9)$$

where l_1+l_2+l = even and l has the value of 0, 2, 4.

$$f(2,2,l,R) = \frac{4\pi}{2\ l+1} \sum_{m_1=-2}^{2} C(2\ 2\ l, m_1 m_1, o)\, 4\pi\, X^{22m} (-1)^{2+m} \qquad (7\text{-}10)$$

Figure 7.2 shows $\omega_1 = (\theta_1, \phi_1)$ and $\omega_2 = (\theta_1, \phi_{12})$.

Figure 7.3 shows the effect of the quadrupole moment on a subspace of angular pair correlation function.

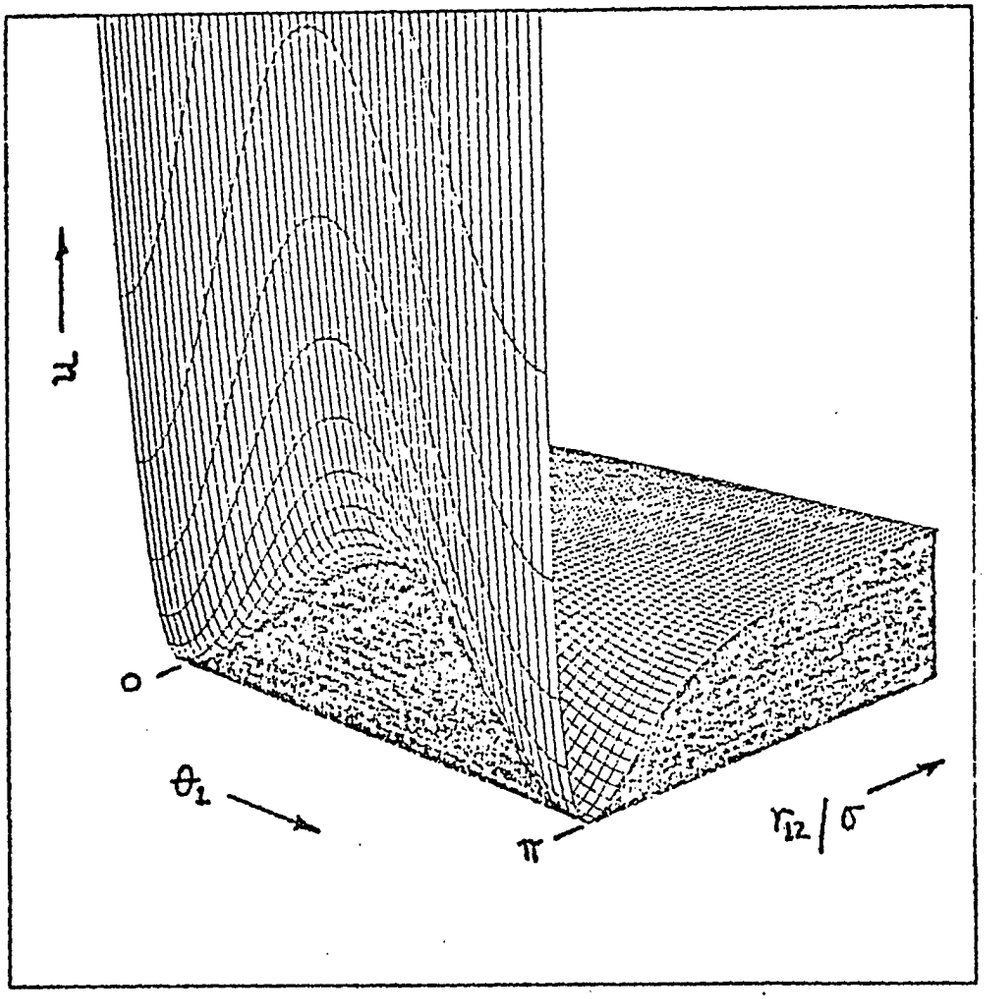


Figure 7.3 Surface of intermolecular pair potential $u(r_{12}\theta_1\theta_2\phi)$ for linear molecule modeled by Lennard-Jones plus quadrupole interaction. $Q/(\varepsilon\sigma^5)^{\frac{1}{2}}=1$. θ_2 is fixed at $\pi/2$ and ϕ is undefined.

CHAPTER VIII

CALCULATION

As we mentioned before, we can write

$$\frac{Y(12)}{Y^{o}(12)} = 1 + \rho\Omega^{-1}\int d3h(13)g^{o}(32)f(32) \qquad (8\text{-}1)$$

or

$$\frac{Y(12)}{Y^{o}(12)} = 1 + \rho\int dR_{13}\Omega_{13}\langle hg^{o}f\rangle_{\omega_3}R_{13}^{2} \qquad (8\text{-}2)$$

Now we can expand; in the space fixed spherical harmonic

$$\frac{Y}{Y^{o}} = \sum_{\substack{\bar{l}_1\\ \bar{l}_2\\ \bar{l}}}\sum_{\substack{\bar{m}_1\\ \bar{m}_2\\ \bar{m}}}\sum_{\substack{\bar{n}_1\\ \bar{n}_2}} E_{Y}(\bar{l}_1\bar{l}_2\bar{l}\ n_1\ ,n_2\ ,R_{12})C(\bar{l}_1\bar{l}_2\bar{l},\ \bar{m}_1\bar{m}_2\bar{m})\cdot \qquad n_1 = n_2 = 0$$

$$Y_{\bar{l}_1}^{\bar{m}_1^{*}}(\omega_1)Y_{\bar{l}_2}^{\bar{m}_2^{*}}(\omega_2)Y_{\bar{l}}^{\bar{m}}(\Omega_{12}) \qquad (8\text{-}3)$$

Expanding h (total correlation function)

$$h = \sum_{\substack{l_1\\ l_3\\ l}}\sum_{\substack{m_1\\ m_3\\ m}}\sum_{\substack{n_1\\ n_3}} E_{h}(l_1l_3l,n_1\ ,n_3\ ,R_{13})C(l_1l_3l,m_1m_3m)\cdot \qquad n_1 = n_3 = 0$$

$$Y_{l_1}^{m_1^{*}}(\omega_1)Y_{l_3}^{m_3^{*}}(\omega_3)Y_{l}^{m}(\Omega_{13}) \qquad (8\text{-}4)$$

Also, we expand f in the space fixed spherical harmonic

$$f = \sum_{\substack{l_3' \\ l_2' \\ l'}} \sum_{\substack{m_3' \\ m_2' \\ m'}} \sum_{\substack{n_3' \\ n_2'}} E_f(l_3', l_2', l', n_3, n_2 R_{32}) C(l_3' l_2' l, m_3' m_2' m') \cdot$$

$$Y_{l_3'}^{m_3'*}(\omega_3) Y_{l_2'}^{m_2'*}(\omega_2) Y_{l'}^{m'}(\Omega_{32}) \qquad (8\text{-}5)$$

Furthermore, we can write

$$\langle hg^0 f \rangle_{\omega_3} = \sum \frac{(-1)^{m_1'}}{4\pi} \delta_{l_3 l_3'} \delta_{m_3 \bar{m}_3} E_h E_f(l_1 l_3 l m_1 m_3 m)$$

$$C(l_3 l_2 l\ m_3 m_2' m') Y_{l_1}^{m_1^*}(\omega_1) (Y_{\ell_2}^{m_2'}(\omega_2) Y_{\ell_1}^{m_1'}(\Omega) g^0 \qquad (8\text{-}6)$$

The terms are non zero only when $l_3 = l_3^1$, $m_3 = m_3^1$ and since

$$\frac{1}{\Omega}\int d\omega_3\ Y_{l_3}^{m_3^*}(\omega_3) Y_{l_3'}^{m_3'*}(\omega_3) = \frac{1}{\Omega}\int d\omega_3\ Y_{l_3}^{m_3^*}(-1)^{m_3'} Y_{\ell_3'}^{m_3'}$$

$$= \frac{1}{4\pi}(-1)^{m_3} \delta_{\ell_3 \ell_3'} \delta_{m_3 \bar{m}_3'} \qquad *8\text{-}7)$$

$$Y_l^{m*}(\theta, \phi) = (-1)^m Y_l^{\bar{m}}(\theta, \phi)$$

Substituting in

$$\frac{Y}{Y^0} = 1 + \frac{1}{4\pi}\int dR_{13} d\Omega_{13} R_{13}^2 \sum_{\substack{l_1 \\ l_3 \\ l}} \sum_{\substack{l_1 \\ l_3 \\ l}} \sum_{\substack{m_1' \\ m_2' \\ m'}} E_h(l_1 l_3 l\ R_{13}) C(l_1 l_3 l, m_1 m_3 m) \cdot$$

$$Y_{l_1}^{m_1^*}(\omega_1)Y_{\ell}^{m}(\Omega_{13})g_o \; f(l_3 l_3' l', R_{32})C(l_3 l_2' l_1', -m_3 m_2' m_1') \cdot \qquad (8\text{-}9)$$

$$Y_{l_2'}^{m_2'^*}(\omega_2)Y_{l_1}^{m'}(\Omega_{32}) \; (-1)^{m_3}$$

CHAPTER IX

MODEL

In the space fixed coordinate, the three molecules 1, 2, 3 can be shown as in Figure 9.1 with the polar coordinate of R_1, R_2, R_3 and (θ_1, ϕ_1), (θ_2, ϕ_2),

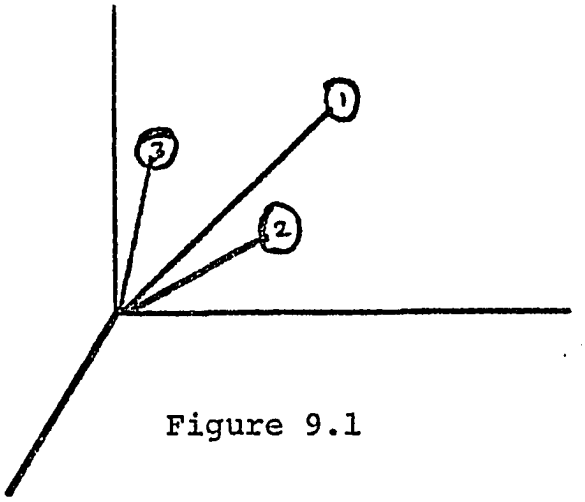


Figure 9.1

or we can simply fix our coordinates such that the origin is on molecule 1 and one axis passes through molecule 2. So Figure 9.1 can be simplified as Figure 9.2.

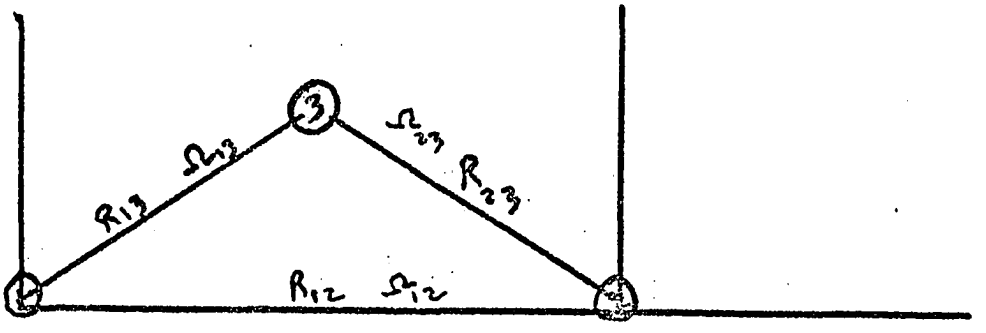


Figure 9.2

Since molecule 1 is always on the origin, new coordinate would be (R_{13},Ω_{13}) and also (R_{12}, Ω_{12}). Furthermore, (R_{12}, R_{13}) remains constant and Ω_{12}, R_{23}, Ω_{23} would be the only variable factors. In other words, we have to calculate R_{23}, Ω_{23} by knowing Ω_{12} and the constants. Let us call $\Omega_{12} = (\theta_2,\phi_2)$ and $\Omega_{23} = (\theta_3,\phi_3)$. Let us represent $\underset{\sim}{R}_{23}$, $\underset{\sim}{R}_{13}$, $\underset{\sim}{R}_{12}$ by vector components so

$$\underset{\sim}{R}_{23} = (v_1,v_2,v_3)$$

$$\underset{\sim}{R}_{13} = (w_1,w_2,w_3) \qquad (9\text{-}1)$$

$$\underset{\sim}{R}_{12} = (u_1,u_2,u_3)$$

$$(w_1-u_1) = (v_1)$$

$$\underset{\sim}{R}_{23} = (w_2-u_2) = (v_2) \qquad (9\text{-}2)$$

$$(w_3-u_3) = (v_3)$$

but from the geometry we have

$$w_1 = R_{13}\text{Sin } \theta_{13} \text{ Cos } \phi_{13}$$

$$w_2 = R_{13}\text{Sin } \theta_{13} \text{ Sin } \phi_{13} \qquad (9\text{-}3)$$

$$w_3 = R_{13}\text{Cos } \theta_{13}$$

also, by similarity, one can write

$$u_1 = R_{12}\text{Sin } \theta_{12} \text{ Cos } \phi_{12}$$

$$u_2 = R_{12}\text{Sin } \theta_{12} \text{ Sin } \phi_{12}$$

$$u_3 = R_{12}\text{Cos } \theta_{12} \qquad (9\text{-}4)$$

and

$$v_1 = R_{23}\text{Sin } \theta_{23} \text{ Cos } \phi_{23}$$

$$v_2 = R_{23}\text{Sin } \theta_{23} \text{ Sin } \phi_{23}$$

$$v_3 = R_{23} \text{ Cos } \theta_{23} \tag{9-5}$$

From this last set of equations we can have

$$R_{23} = \frac{w_1-u_1}{\text{Sin } \theta_{23} \quad \phi_{23}} = \frac{w_3-u_3}{\text{Cos } \theta_{23}} = \frac{R_{13} \text{Cos } \theta_{13}-R_{12} \text{ Cos } \theta_{12}}{\text{Cos } \theta_{23}}$$

$$\text{Cos } \theta_{23} = \frac{w_3-u_3}{R_{23}} \tag{9-6}$$

and

$$R_{23} = (w_1-u_1)^2 + (w_2-u_2)^2 + (w_3-u_3)^2 \tag{9-7}$$

$$\text{Cos } \phi_{23} = \frac{w_1-u_1}{R_{23} \text{ Sin } \theta_{23}} \text{ or } \text{Sin } \phi_{23} = \frac{w_2-u_2}{R_{23} \text{ Sin } \theta_{23}} \tag{9-8}$$

$$R_{13}^2 = w_1^2 + w_2^2 + w_3^2$$

$$\text{Cos } \theta_{13} = \frac{w_2}{R_{13}}$$

$$\text{Sin } \theta_{13} = \frac{(w_1^2 + w_2^2)^{\frac{1}{2}}}{R_{13}}$$

$$\text{Cos } \phi_{13} = \frac{w_1}{(w_1^2 + w_2^2)^{\frac{1}{2}}} \tag{9-9}$$

$$\text{Sin } \theta_{13} \text{ Cos } \theta_{13} = \frac{w_1}{R_{13}}$$

$$\text{Sin } \phi_{13} = \frac{w_2}{(w_1^2 + w_1^2)^{\frac{1}{2}}}$$

so $\text{Sin}\ \theta_{13}\ \text{Sin}\ \theta_{13} = \dfrac{w_1}{R_{13}}$

but $R_{32}^2 = (w_1-u_1)^2 + (w_2-u_2)^2 + (w_3-u_3)^2$ (9-10)

and also

$$\text{Cos}\ \theta_{12} = \frac{u_3}{R_{12}} \tag{9-11}$$

$$\text{Sin}\ \theta_{12} = \frac{(u_1^2+u_2^2)^{\frac{1}{2}}}{R_{12}} \tag{9-12}$$

$$\text{Cos}\ \phi_{12} = \frac{u_1}{(u_1^2+u_2^2)^{\frac{1}{2}}} \tag{9-13}$$

$$\text{Sin}\ \phi_{12} = \frac{u_2}{(u_1^2+u_2^2)^{\frac{1}{2}}} \tag{9-14}$$

$$\text{Sin}\ \theta_{12}\ \text{Cos}\ \theta_{12} = \frac{u_2}{R_{12}} \tag{9-15}$$

$$\text{Sin}\ \theta_{12}\ \text{Sin}\ \phi_{12} = \frac{u_2}{R_{12}} \tag{9-16}$$

For Ω_{23}

$$\text{Cos}\ \theta_{23} = \frac{w_3-u_3}{R_{23}} \tag{9-17}$$

$$\text{Sin}\ \theta_{23} = \frac{[(w_1-u_1)^2+(w_2-u_2)^2]^{\frac{1}{2}}}{R_{23}} \tag{9-18}$$

$$\text{Cos}\ \phi_{23} = \frac{w_1-u_1}{[(w^2-u_1)^2+(w_2-u_2)^2]^{\frac{1}{2}}} \tag{9-19}$$

$$\text{Sin } \phi_{23} = \frac{w_2-u_2}{[(w_1-u_1)^2+(w_2-u_2)^2]^{\frac{1}{2}}} \tag{9-20}$$

And finally,

$$\text{Sin } \theta_{23} \text{ Cos } \phi_{23} = \frac{w_1-u_1}{R_{23}}$$

$$\text{Sin } \theta_{23} \text{ Sin } \phi_{23} = \frac{w_1-u_1}{R_{23}} \tag{9-21}$$

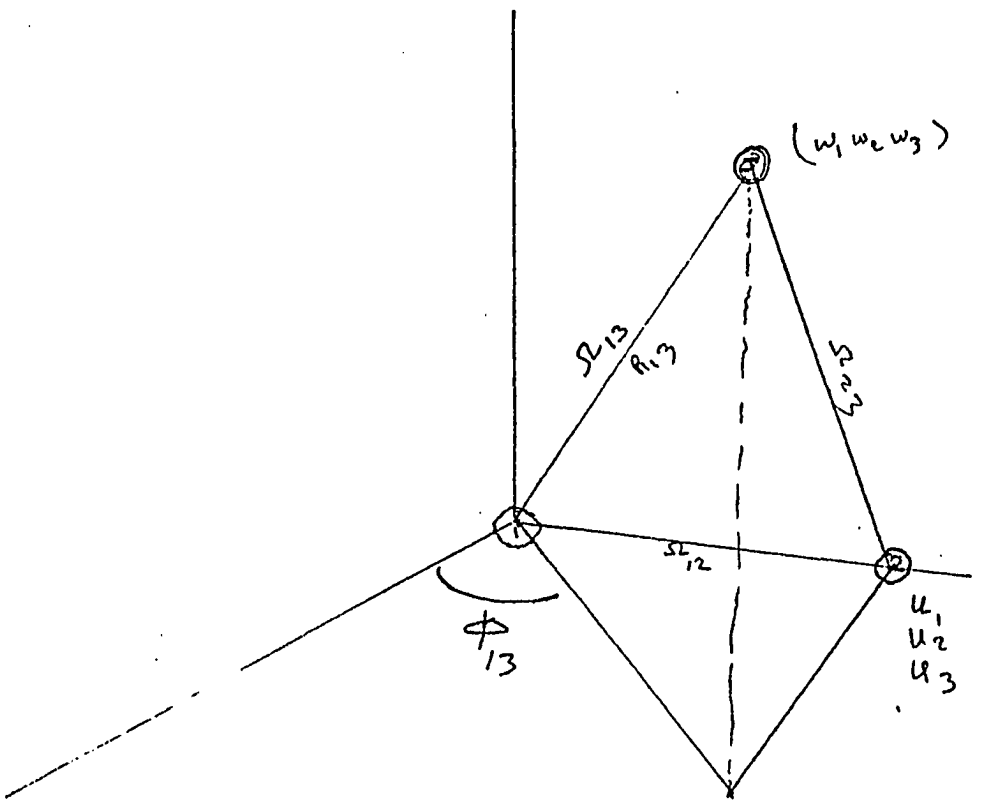


Fig 9-3

CHAPTER X

PROCEDURE

First we had to find $F = \exp(-\beta u)-1$, so called Mayer function. The spherical harmonic expansion of F in the space fixed coordinate is

$$F(r,\omega_1\omega_2)= \sum_{\substack{l_1\ m_1\\ l_2\ m_2\\ l\ m}} E_f(l_1l_2l,r)C(l_1l_2l,m_1m_2m)Y_{l_1}^{m_1}(\omega_1)Y_{l_2}^{m_2}(\omega_2)Y_l^{m*}(\Omega) \tag{10-1}$$

where $E_f(l_1l_2l,r)$ are the expansion coefficients and by orthogonality condition of $C(l_1l_2l,m_1m_2m)$ which has been mentioned before, and also because of the orthogonality of spherical harmonics function

$$\int d\omega_1 Y_l^m(\omega_i)\ Y_{l'}^{m'*}(\omega_1) = \delta_{ll}\ \delta_{m'm} \tag{10-2}$$

we can write

$$E_f(l_1l_2l,r) = \int_o^\pi d\theta_1 \int_o^\pi d\theta_2 \int_o^\pi d\theta_3 \int_o^{2\pi} d\phi_1 \int_o^{2\pi} d\phi_2 \int_o^{2\pi} d\phi_3 F(r,\omega_1,\omega_2)\cdot$$

$$C(l_1l_2l,m_1m_2m)Y_{l_1}^{m_1}(\omega_1)Y_{l_2}^{m_2^*}(\omega_2)Y_l^m(\Omega) \tag{10-3}$$

This is a six fold integral.

Integration

Since this multidimensional integral cannot be evaluated by analytical means, numerical integration processes must be used. The methods generally employed are based on the product of Simpson's rule or the product of Gaussian formulae. While these formulae can be applied to give the value of a multiple integral correct to any accuracy, they are not the most economical formulae in the sense that a large number of integrand function evaluations is needed. Since these evaluations are the most time-consuming part of these computations, economy is an important factor. Integration formulae which are exact for multinomials over the entire region of integration are necessarily more economical than the product formulae and can be applied to the same accuracy by subdividing the integration region.

The construction of a satisfactory multidimensional non-product formula for a given hyper-region is a matter of some difficulty and is in fact a problem in the theory of algebraic equations.

The required formula must have positive weights associated with it in order to avoid loss of accuracy by cancellation and all the integration points must lie entirely within the integration region. Watts has given a general third degree formula valid for the hypercube of side 2 and centered on the origin. Let $\Sigma_n(k)$ denote the point $(\sigma_1^{(k)}, \sigma_2^{(k)} \ldots\ldots \sigma_n^{(k)})$ of the n-dimensional Euclidean space, σ^n, for k=1, 2, ...2n

and

$$\sigma_{2S-1}^{(k)} = (2/3)^{\frac{1}{2}} \quad \text{Cos} \quad (2S-1)\ \frac{k\pi}{n}$$

$$\sigma_{2S}^{(k)} = (2/3)^{\frac{1}{2}} \quad \text{Sin} \quad (2S-1)\ \frac{k\pi}{n} \qquad (10\text{-}4)$$

where $S = 1,2,\ldots\ \ldots n/2$, and when n is odd $\sigma_n^{(k)} = (-1)^k/\sqrt{3}$. If S_n be the hypercube of side 2 and the center at the origin an integral over S_n may be evaluated by the formula.

The weight for each point is 1/2n. We also used shifting methods to get a more accurate answer. This method could cut the computer time, except that in this 6-fold integral $f = \exp(-\beta u)-1$, where u itself must be expanded in the space fixed coordinate and again is 6-fold integral.

With shifting twice within 6 dimensions, we had to calculate one point (n+2)*(n+2) which is 64 summations and still the accuracy was poor. So what we decided was as follows. We calculated these coefficients of expansion in the body fixed, then transferred them to the space fixed coordinate by transformation formula (4-2). The spherical harmonic expansion of the Mayer function in the body fixed coordinate is

$$F(r_{12},\omega_1,\omega_2) = 4\pi \sum_{\substack{l_1 \\ l_2 \\ m_1}} E_f(l_1 l_2 m_1 r_{12}) Y_{l_1}^{m_1}(\omega_1) Y_{l_2}^{\underline{m}_1}(\omega_2) \qquad (10\text{-}5)$$

The $g(l_1 l_2 m, r_{12})$ are the expansion coefficients to be determined. For molecules with a plane of symmetry perpendicular to the molecular axis, the $E_f(l_1 l_2 m_1 r_{12})$ are zero unless

both l_1 and l_2 are even (homonuclear diatomics e.g.). For heteronuclear diatomics $E_f(l_1 l_2 mr)$ both odd and even values contribute. Multiplying both sides of (10-5) by $Y_{l_1}^{m*}(\omega_1)$ $Y_{l_2}^{\bar{m}*}(\omega_2)$ where * indicates complex conjugate and integrating over ω_1 and ω_2

$$\int d\omega_1 d\omega_2 g(r_{12},\omega_1,\omega_2) Y_{l_1}^{m*}(\omega_1) Y_{\ell_2}^{\bar{m}*}(\omega_2) = 4\pi \sum_{l_1 l_2 m} E_g(l_1 l_2 m, r_{12}) \cdot \quad (10\text{-}6)$$

$$\int d\omega_1 Y_{l_1}^{m}(\omega_1) Y_{l_1}^{m*}(\omega_1) \int d\omega_2 Y_{l_2}^{\bar{m}}(\omega_2) Y_{l_2}^{\bar{m}_1*}(\omega_2)$$

but $\int d\omega Y_l^m(\omega) Y_{l_1}^{m'*}(\omega) = \delta_{ll'} \delta_{mm'}$

$$E_g(l_1 l_2 m, r_{12}) = \frac{1}{4\pi} \int d\omega_1 d\omega_2 Y_{l_2}^{\bar{m}*}(\omega_2) g(r_{12},\omega_1,\omega_2) \qquad (10\text{-}7)$$

Dividing both sides of (10-7) by $\int d\omega_1 \, d\omega_2 \, g(r_{12}\omega_1\omega_2)$

$$\frac{E_g(l_1 l_2 m, r_{12})}{\int d\omega_1 d\omega_2 g(r_{12},\omega_1,\omega_2)} = \frac{1}{4\pi} \frac{\int d\omega_1 d\omega_2 Y_{l_1}^{m*}(\omega_1) Y_{l_2}^{\bar{m}*}(\omega_2) g(r_{12},\omega_1,\omega_2)}{\int d\omega_1 d\omega_2 g(r_{12}\omega_1\ \omega_2)}$$

(10-8)

where $\bar{m}_1 = -m_1$

and

$$Y_l^m(\omega) = Y_l^m(\theta,\phi) \qquad (10\text{-}9)$$

We can write the formula for $g(r_{12},\omega_1,\omega_2)$ with the same form of expansion coefficient so we have equation (10-7) in terms of

$$g(r_{12}\omega_1\omega_2) = 4\pi \sum_{l_1 l_2 m} g(l_1 l_2 m, r_{12}) Y_{l_1}^{m}(\omega_1) Y_{l_1}^{\bar{m}}(\omega_2) \qquad (10\text{-}10)$$

The average of a property $X(r_{12},\omega_1,\omega_2)$ in a spherical shell of radius between r_{12} and $r_{12}+dr_{12}$ is defined by

$$\langle X(r_{12},\omega_1\omega_2)\rangle_{shell} = \frac{\int d\omega_1 d\omega_2 X(r_{12},\omega_1,\omega_2) g(r_{12},\omega_1,\omega_1)}{\int d\omega_1\, d\omega_2\, g(r_{12},\omega_1,\omega_2)} \quad (10\text{-}11)$$

Further, from (10-7) we have

$$g_{ooo}(r_{12}) = \frac{1}{(4\pi)} \int d\omega_1 d\omega_2\, g(r_{12},\omega_1,\omega_2)$$

Combine (10-10) and (10-11) to give

$$Y(l_1 l_2 m\, r_{12}) = 4\pi\, g_{ooo}(r_{12}) \langle Y_{l_1}^{m_1^*}(\omega_1) Y_{l_2}^{\bar{m}_1^*}(\omega_2)\rangle \text{ shell} \quad (10\text{-}12)$$

Note this $g_{ooo}(r)$ is the same $g_o(r)$ expression for all $g(l_1,l_2 m r_{12})$ having l_1 and l_2 even up to $\{l_1,l_2,m\} = \{4,4,4\}$ and the additional terms with ℓ_1 and ℓ_2 even, m = o to $\{l_1 l_2 m = \{800\}$ are tabulated in Appendix F of Reference 1.

We had used the data of $g_{ooo}(r)$ from Verlet where r_{12} goes from 0.7 up to 3.2.(We found the g_{ooo} for higher r_{12} by extrapolation.)

Calculation of g_oF

As mentioned before, to calculate the expansion coefficients of the F in the body fixed coordinate, we used Simpson's rule to solve multiple integral. Since $\phi_2 = 0$

$$E_f(l_1 l_2 m, r_{12}) = \int d\theta_1 \int d\theta_2 \int d\theta_1 F(r_{12},\omega_1,\omega_2) Y_{l_1}^{m_1}(\omega_1) Y_{\ell_2}^{\bar{m}}(\omega_2) \quad (10\text{-}13)$$

$\omega_1 = (\theta_1, \phi_1)$, $\omega_2 = (\theta_2, o)$

and $F(r_{12}, \omega_1, \omega_2) = \exp(-\beta u(r_{12}, \omega_1, \omega_2)) - 1$

The potential U has been discussed before. $\beta = 1/kT$ where k is the Boltzmann constant. This evaluation has been carried out for two different conditions: $T^* = 1.277$ and $Q = 0.5$; $T^* = 1.294$ and $Q = 1$. Q is the quadrupole moment discussed in the potential chapter.

The $Y_l^m(\omega)$ spherical harmonic functions have been calculated from $l = 0$ to $l = 4$ and in each calculation it has been fit in.

By finding the coefficients of $E_f(l_1 l_2 m_1 r_{12})$ and using the conversion from body to spaced fixed coordinates, we could find the $E_f(l_1 l_2 l, r_{12})$ where $|l_1 - l_2| \leq l \leq (l_1 + l_2)$ and later we were able to find $g^o(r_{12}) * E_f(l_1 l_2 l r_{12})$ for each r_{12} from 0.7 to 3.2 with dr = 0.04 when g_o is at reduced density of 0.85. Pages 55 to 67 show some results for E_f.

After having reduced the $g^o E_f(l_1 l_2 l, r_{12})$ for reduced density of 0.85 and two different temperatures and quadrupole moments, we are able to calculate the $E_f(l_1 l_2 l, r_{12})$ and the space fixed spherical harmonic expansion coefficients of direct correlation function $h(r_{12}, \omega_1, \omega_2)$. Simulation results are given by Dr. Haile in his dissertation (7) for $l_1 = 0$ to 4, $l_2 = 0$ to 4 and m going from negative of l_1 or l_2 up l_1 or l_2 depending on which one is smaller.

Now since

$$g(l_1 l_2\ m\ R_{12}) = h(l_1 l_2\ m\ R_{12}) - 1$$

by transferring the body fixed to space fixed coordinates, we were able to calculate all $E_g(l_1 l_2 l, r_{12})$ from $l_1 = 0$ to 4 and $l_2 = 0$ to 4 for r starting from 0.7 up to 3.2 with dr = 0.025. The only difference here is the dr in both coefficients of $E_f(l_1 l_2 l, r_{12})$ and $E_h(l_1 l_2 l\ r_{12})$ which we took care of by changing our dr from 0.04 to 0.025. In Table 1.2, some values for $g(l_1 l_2\ m\ r_{12})$ and $g(l_1 l_2 l\ r_{12})$, $E_h(l_1 l_2 l\ r_{12})$ are given.

CHAPTER XI

CONVOLUTION PART B

We can arrange the formula for Y and write

$$\left(\frac{Y(12)}{Y_o(n)} - 1\right) = \sum_{\substack{\bar{l}_1 \\ l_2}} \sum_{\substack{\bar{m}_1 \\ \bar{m}_2 \\ m}} E_Y(\bar{l}_1\bar{l}_2,\bar{l},R_{12})C(\bar{l}_1\bar{l}_2,\bar{l},\bar{m}_1,\bar{m}_2m) \cdot$$

$$Y_{l_1}^{\bar{m}_1}(\omega_1)Y_{l_2}^{\bar{m}_2}(\omega_2)Y_1^{m*}(\Omega_{12}) \qquad (11\text{-}1)$$

Also for h (13), we had

$$h(13) = \sum_{\substack{l_1 \\ l_3 \\ l}} \sum_{\substack{m_1 \\ m_3 \\ m}} E_h(l_1l_2l,R_{13})C(l_1l_3l,m_1m_3m)Y_{l_1}^{m_1}(\omega_1)Y_{l_3}^{m_3}(\omega_2) \cdot$$

$$Y_1^m(\Omega_{13}) \qquad (11\text{-}2)$$

For $g^oF(23)$, we can write

$$g^oF(23) = \sum_{\substack{l_3' \\ l_2' \\ l'}} \sum_{\substack{m_3' \\ m_2' \\ m'}} E_f(l_3'l_2'l',R_{32})C(l_3'l_2',m_3'm_2'm') \qquad (11\text{-}3)$$

$$Y_{l_3'}^{m_3'}(\omega_3)Y_{l_2'}^{m_2'}(\omega_2)Y_{l_1'}^{m'*}(\Omega_{32})$$

Now we substitute for $g^of(23)$ and h(13) to get $\langle h^*(13)g^of(23)\rangle_{\omega_3}$.

By definition of $\langle \ldots\ldots \rangle_{\omega_3}$ and using the orthogonality condition for both spherical harmonic functions and Clebsch Gordon coefficients, we have

$$\langle h^*(13) g^{o} f(23) \rangle_{\omega_3} = \int d\omega_3 \sum_{\substack{l_1 \\ l_3 \\ l}} \sum_{\substack{m_1 \\ m_3 \\ m}} E_h(l_1 l_3 l, R_{13}) C(l_1 l_3 l, m_1 m_3 m)$$

$$Y^{m_1^*}_{l_1}(\omega_1) Y^{m_3^*}_{l_3}(\omega_3) Y^{m}_{l}(\Omega_{13}) \sum_{\substack{l_3' \\ l_2' \\ l'}} \sum_{\substack{m_3' \\ m_2' \\ m'}} E_f(l_3' l_2' l', R_{32}) \qquad (11\text{-}4)$$

$$C(l_3' l_2' l' m_3' m_2') Y^{m_3'}_{l_3'}(\omega_3) Y^{m_2'}_{l_2'}(\omega_2) Y^{m'*}_{l'}(\Omega_{32})$$

Since

$$\int d\omega_3 Y^{m_3'}_{l_3'}(\omega_3) Y^{*}_{l_3 m_3}(\omega_3) = \frac{1}{4\pi} \delta_{l_3' l_3} \delta_{m_3' m_3} \qquad (11\text{-}5)$$

The only non-zero term will be when $l_3' = l_3$ and $m_3' = m_3$ and the average will be

$$\langle h^*(13) g^{o} f(23) \rangle_{\omega_3} = \frac{1}{4\pi} \sum_{\substack{l_1 \\ l_3 \\ l}} \sum_{\substack{m_1 \\ m_3 \\ m}} \sum_{\substack{l_2' \\ l' }} \sum_{\substack{m_2 \\ m'}} E_h(l_1 l_3 l, R_{12})$$

$$E_f(l_3 l_2 l R_{12}) C(l_3 l_2 l, m_3 m_2 m) C(l_1 l_2' l' m_1 m_2' m) \qquad (11\text{-}6)$$

$$Y^{m_1^*}_{l_1}(\omega_1) Y^{m}_{l}(\Omega_{13}) Y^{m_2'}_{l_2'}(\omega^2) Y^{m_*'}_{l'}(\Omega_{32})$$

Furthermore, we also had for

$$\frac{Y}{Y_o} = 1 + \int\int dR_{13} d\Omega_{13} \langle h^* g^o f \rangle_{\omega_3} R_{13}^2$$

or by substitution for

$$\langle h^* g^o f \rangle_{\omega_3}$$

$$\frac{Y(12)}{Y^o} - 1 = \frac{\rho}{4\pi} \int dR_{13} R_{13}^2 d\theta_{13} \sin\theta_{13} d\phi_{13} \sum_{\substack{l_2' \\ l'}} \sum_{\substack{l_1 \\ l_3 \\ l}} \sum_{\substack{m_2' \\ m \\ m}} \sum_{\substack{m' \\ m^3 \\ m}}$$

$$E_h(l_1 l_3 l, R_{13}) C(l_1 l_3 l m_1 m_3 m) Y_{l_1}^{m_1^*}(\omega_1) Y_{l_2'}^{m_2'}(\omega_2) Y_l^m(\Omega_{12}) Y_{l_1}^{m'*}(\Omega_{32}) \cdot$$

$$C(l_3 l_2' l' m_3 m_2' m') \qquad (11\text{-}7)$$

From this equation one can have

$$\int d\omega_1 Y_{L_1}^{M_1}(\omega_1) \left(\frac{Y(12)}{Y_o(12)} - 1\right) = \sum_{\substack{\bar{l} \\ \bar{l}_2}} \sum_{\substack{\bar{m} \\ \bar{m}_2}} E_Y(L_1 \bar{l}_2 \bar{l}, R_{12}) \cdot$$

$$C(L_1 \bar{l}_2 \bar{l}\ \underline{M}_1 \bar{m}_2 \bar{m}) Y_{\bar{l}_2}^{\bar{m}_2}(\omega_2) Y_{\bar{l}}^{\bar{m}^*}(\Omega_{12}) (-1)^{M_1} \qquad (11\text{-}8)$$

$$\bar{l}_1 = L_1$$

$$\bar{m}_1 = \underline{M}_1$$

where $\underline{M}_1 = -M_1$.

So one can substitute for the left hand side of (11-8) and integrate over $d\omega_2$. The non-zero terms occur when

$$l_1 = L_1$$

$$m_1 = M_1$$

$$\frac{\rho}{4\pi} \int dR_{13} R_{13}^2 d\theta_{13} \operatorname{Sin}\theta_{13} d\phi \sum_{l'} \sum_{l_3} \sum_{m_3} \sum_{m_2'} E_h(L_1 l_3 l, R_{13}) \cdot$$
$$l_2' \quad l \quad m \quad m'$$

$$C(L_1 l_3 M_1 m_3 m) Y_{l_2'}^{m_2'}(\omega_2) Y_l^m(\Omega_{12}) Y_{l'}^{m'*}(\Omega_{32}) \qquad (11\text{-}9)$$

Again we can multiply equation (11-8) by $Y_{L_2}^{m_2^*}(\omega_2)$ and integrate over $d\omega_2$ to have

$$\int d\omega_2 Y_{L_2}^{M_2^*}(\omega_2) \int d\omega_1 \; Y_{L_1}^{M_1}(\omega_1) \left(\frac{Y}{Y_o} - 1\right) = \qquad (11\text{-}10)$$

$$\sum_{\bar{l}} \sum_{\bar{m}} E_Y(L_1 L_2 \bar{l}, R_{12}) C(L_1 L_2 \bar{l}, \underline{M}_1 M_2 \bar{m}) Y_{\bar{l}}^{\bar{m}*}(\Omega_{12}) (-1)^{M_1}$$

which gave us $\bar{l}_2 = L_2$ and $\bar{m}_2 = M_2$. Substituting in (11-7) we have on the R.H.S.

$$\frac{\rho}{4\pi} \int dR_{13} R_{13} \operatorname{Sin}\theta_{13} d\phi_{13} \sum_{\substack{l_3 \\ l}} \sum_{\substack{m_3 \\ m}} \sum_{l'} \sum_{m'} E_h(L_1 l_3 l, R_{13}) Y_l^m(\Omega_{13}) \cdot$$

$$Y_{l'}^{m'*}(\Omega_{32}) E_f(l_3 L_2 l', R_{32}) C(l_3 L_2 l', m_3 M_2 M') \qquad (11\text{-}11)$$

where $l_2' = L_2$

$$m_2' = M_2$$

Again on the R.H.S. of equation (11-10) we have

$$(-1)^{M_1} \sum_{\bar{l}} \sum_{\bar{l}} E_Y(L_1 L_2 \bar{l}, R_{12}) C(L_1 L_2 \bar{l}, \underline{M}_1 M_2 \bar{m}) Y_{\bar{l}}^{\bar{m}*}(\Omega_{12}) \qquad (11\text{-}12)$$

When we multiply both sides of equation (11-12) by $Y_L^M(\Omega_{12})$ and integrate over Ω_{12}, we have

$$\int d\Omega_{12} Y_L^M(\Omega_{12}) \int d\omega_2 Y_{L_2}^{M_2}(\omega_2) \int d\omega_1 Y_{L_1}^{M_1}(\omega_1) \left(\frac{Y}{Y_1} - 1\right) =$$

$$(-1)^{M_1} E_Y(L_1 L_2 L, R_{12}) C(L_1 L_2 L, \underline{M}_1 M_2 M) \qquad (11\text{-}13)$$

where here again $\bar{l} = L$ and $\bar{m} = M$. And from equation (11-11) the R.H.S. gives

$$\frac{\rho}{4\pi} \int dR_{13} R_{13} d\theta_{13} \sin\theta_{13} d\phi_{13} d\theta_{12} \sin\theta_{12} d\phi_{12} \cdot$$

$$\sum_{l_3} \sum_{m_3} \sum_{l'} \sum_{m'} E_h(L_1 l_3 l, R_{13}) E_f(l_3 L_2 l', R_{32}) \cdot$$

$$C(L_1 l_3 l, M_1 m_3 m) C(l_3 L_2 l', m_3 M_2 m') Y_l^m(\Omega_{13}) Y_{\ell}^{m'}(\Omega_{32}) \cdot$$

$$Y_L^M(\Omega_{12}) \qquad (11\text{-}14)$$

Finally, the result would be

$$(-1)^{M_1} E_Y(L_1 L_2 L, R_{12}) C(L_1 L_2 L, M_1 M_2 M) =$$

$$\frac{\rho}{\pi} \int dR_{13} R_{13} d\theta_{13} \sin\theta_{13} d\phi_{13} d\theta_{12} \sin\theta_{12} d\phi_{12} \cdot$$

$$\sum_{l_3}\sum_{m_3}\sum_{l'}\sum_{m'}\sum_{l} E_h(L_1 l_3 l, R_{13}) E_f(l_2 L_3 l', R_{32}) \cdot$$

$$C(L_1 l_3 l, M_1 m_3 m) C(l_3 L_2 l', m_3 M_2 m') Y_\ell^m(\Omega_{13}) \cdot$$

$$Y_{l'}^{m'*}(\Omega_{32}) Y_L^M(\Omega_{12})$$

This is a 5 fold integral which must be computed by computer.

$$RHS = \sum_{\bar{l}}\sum_{\bar{m}} E_Y(L_1 L_2 \bar{l} R_{12}) C(L_1 L_2 \bar{l} M_1 M_2 \bar{m})$$

$$(-1)^{M_1} Y_{\bar{l}}^{\bar{m}*}(\Omega_{12}) = \sum_{m}\sum_{\bar{l}} E_Y(L_1 L_2 \bar{l} R_{12}) C(L_1 L l M_1 M_2 \bar{m}) \cdot$$

$$(-1)^{M_1} \left(\frac{2l+1}{4\pi}\right)^{\frac{1}{2}} \left(\frac{(\bar{l}-\bar{m})!}{(\bar{l}+\bar{m})!}\right)^{\frac{1}{2}} e^{iM\phi} P_l^{\bar{m}}(\chi = \cos\theta)$$

$$= \frac{\rho}{4\pi} \int dR_{13} R_{13} d\theta_{13} \sin\theta_{13} d\phi_{13} \sum_{l_3}\sum_{m_3}\sum_{l_1}\sum_{m_1}\sum_{l}\sum_{m} E_h(L_1 \ell_2 \ell R_{13}) \cdot$$

$$C(L_1 l_3 l \underline{M_1} m_3 m)\ E_f(l_3 L_2 l' R_{32}) C(l_3 L_2 l' m_3 M_2 m') \cdot$$

$$Y_l^m(\Omega_{13}) Y_{l'}^{m'*}(\Omega_{32}) (-1)^{M_1}$$

In the special case when

$$\phi_{12} = \frac{\pi}{2}\ ,\ \phi_{12} = 0$$

$$\theta_{12} = \frac{\pi}{2}\ ,\ \theta_{12} = 0$$

$$E_Y(l_1 l_2 m_1 R_{12}) = \frac{1}{4\pi} \sum_{l} \left(\frac{2\,l+1}{4\pi}\right)^{\frac{1}{2}} E_Y(l_1 l_2 l,\ R_{12}) \cdot$$

$$C(l_1 l_2 l\ m_1 \bar{m}_1 o)$$

since $Y_o^o = \left(\frac{1}{4\pi}\right)^{\frac{1}{2}}$

$$Y_1^{-1}\left(\frac{\pi}{2}\ \frac{\pi}{2}\right) = -\left(\frac{3}{8\pi}\right)^{\frac{1}{2}}$$

$$Y_l^m(\theta,\phi) = \left(\frac{2\,\ell+1}{4\pi}\right)^{\frac{1}{2}} \left(\frac{(l-m)!}{(l+m)!}\right)^{\frac{1}{2}} e^{\,im\phi} P_l^m(\chi = \text{Cos}\ \theta)$$

where

$$P_l^m(\chi) = (-1)^m\ \text{Sin}\ \theta)^m \frac{1}{2^l l!} \left(\frac{d}{dx}\right)^{\ell+m} (x^2-1)^l$$

In the case when

$$\begin{cases} \phi_{12} = 0 \\ \theta_{12} = 0 \end{cases}$$

$$Y_{\bar{l}}^{\bar{m}}(\theta_{12},\phi_{12}) = Y_{\bar{l}}^{\bar{m}}(0,0) = \left(\frac{2\,\bar{l}+1}{4\pi}\right)^{\frac{1}{2}} \frac{(\bar{l}-\bar{m})!}{(\bar{\ell}+\bar{m})!} .1. \quad 0$$

for $\bar{m} \neq 0$

For $\phi_{12} = 0 \quad \bar{m} = 0 \quad \theta_{12} = 0$

$M_1 = -M_2, C(L_1 L_2 \bar{\ell} M_1 M_2 0) = C(L_1 L_2 \bar{\ell} M_1 M_1 0)$

But $P_o(x) = 1,$

$P_1(x) = x$

$P_2(x) = \frac{1}{2}(3x^2-1) = 1 \quad \text{as } x = 1$

$P_3(x) = \text{-----}$

So

$$\text{RHS} \rightarrow E_Y(l_1 l_2 \ell\, R_{12}) \rightarrow E_Y(l_1 l_2 m_1 R_{12})$$

$$\frac{\Sigma}{m}\, \overline{m} = -\, \overline{l} + \overline{\ell} = 0 \text{ only}$$

RHS = $4\pi\ E_Y(L_1 L_2 M_1 r_{12})$ for $\phi_{12} = 0$ and $\theta_{12} = 0$, depending on which value of M was chosen.

CHAPTER XII

FOURIER TRANSFORMATION

In the convolution chapter we saw a five fold integral is existing which takes lot of computer time. So we decided to use Fourier transformation in order to cut the time.

Assume

$$B(12) = \frac{Y(12)}{Y_o(r_{12})} - 1. = \sum_{\substack{l' \\ l''}} \sum_{\substack{m' \\ m'' \\ m}} E_Y(l'l''\, l, r_{12}) C(l'l'', m'm''\, m) \cdot$$

$$Y_{l'}^{m'}(\omega_1) Y_{l''}^{m''}(\omega_2) Y_l^{m*}(\Omega_{12}) \tag{12-1}$$

Also

$$B(12) = \frac{Y(12)}{Y_o(r_{12})} - 1 = \rho \int d^{\,3} h(13) g_o f(32)$$

$$= \frac{\rho}{4\pi} \int dx_3\, h(13) = g_o f(32) \tag{12-2}$$

And

$$\tilde{B}(k) = \sum_{l_1 l_2 l} \sum \sum \tilde{E}_Y(l_1 l_2 l, k) \sum_{\substack{m_1 \\ m_2}} C(l_1 l_2 l, m_1 m_2 m) Y_l^m(\theta_k \phi_k) Y_{l_2}^{m_1}(\omega_1) Y_{l_2}^{m_2}(\omega_2)$$

$$\tilde{E}_Y(l_1 l_2 l, k) = i^l (4\pi) \int_o^\infty dr\, r^2 J_l(kr) E_Y(l_1 l_2 l, r) \tag{12-3}$$

where $J_l(kr)$ is the spherical Bessel function and $\tilde{B}(k)$ is the Hankel transformation of B(12).

Now

$$\Sigma\tilde{E}_Y C\ Y_{l_1}^{m_1} Y_{l_2}^{m_2} Y_l^{m*} = \frac{\rho}{4\pi}\ \{(\Sigma\tilde{E}_h(l_1' l_2' l', k) C(l_1' l_2' l', m_1', m_2' m') \cdot$$

$$Y_{l_1'}^{m_1'}(\omega_1) Y_{l_2'}^{m_2'}(\omega_2) Y_{l'}^{m'*}) (\Sigma E_f(l_1'' l_2'' l'', k) C(l_1'' l_2'' l'', k, m_1'' m_2'' m) \cdot$$

$$Y_{l_1''}^{m_2''}(\omega_3) Y_{l_2''}^{m_2''*}(\omega_2) Y_{l''}^{m''}) \} \text{ implies } \begin{matrix} m_1' = m''_1 \\ l_2' = l''_1 \end{matrix}$$

also

$$\int_{\ell} e^{ik\cdot(R_{13}-R_{32})} dR_{12} = \int dR_{12}\ e_1^{ik\cdot R_{13}} - e_1^{ikR_{32}}$$

and

$$\int dR_{13} dR_{12}\ h(13) g^{o} f(32)\ e_1^{ik\cdot R_{13}} - e_1^{ikR_{32}} =$$

$$\int dR_{13} h(13)\ e_1^{ik\cdot R_{13}} \int dR_{32} g^{o} f(32)\ e_1^{-ik\cdot R_{32}}$$

$$= \Sigma\tilde{E}_h(l_1' l_2' l, k) C(l_1' l_2' l', m_1 m_2 m) Y_{l_1'}^{m_1}(\omega_1) Y_{l_2'}^{m_2}(\omega_3) Y_{l_1}^{m*}(\theta_k \phi_k) \cdot$$

$$\Sigma\tilde{E}_f(l_1'' l_2'' l'', k) C(l_1'' l_2'' l_2, m_1'' m_2'' m'') \cdot$$

$$Y_{l_1''}^{m_1''}(\omega_3) Y_{l_2''}^{m_2''}(\omega_2) Y_{l_2}^{m*}(\theta_k \phi_k)$$

Also

$$\sum_{\substack{l\\ \lambda}} \tilde{E}_Y(m\ n\ l,k)C(m\ n\ l,\mu\nu\lambda)Y_m^{\mu}(\omega_1)Y_n^{\nu}(\omega_2)Y_l^{\lambda *}(\hat{k})$$

$$= \frac{\rho}{4\pi}\Big\{ \sum_{\substack{n_1\nu_1\\ l_1\\ \lambda_1}} \tilde{E}_h(m_1 n_1 l_1,k)C(m_1 n_1 l_1,\mu_1\nu_1\lambda_1)Y_{m_1}^{\mu_1}(\omega_1)\cdot$$

$$Y_{l_1}^{\lambda_1 *}(k) \sum_{\substack{l_2\\ \lambda_2}} \tilde{E}_f^*(m_1 n_2 l_2,k)C(n_1 n_2 l_2,\nu_1\nu_2\lambda_2)Y_{n_2}^{\nu_2 *}(\omega_2)\cdot$$

$$Y_{l_2}^{\lambda_2}(\hat{k})\ \Big\} \quad \text{implies} \quad \begin{matrix} m_1 = m & \mu_1 = \mu \\ n_2 = n & -\nu_2 = \nu \end{matrix}$$

Since

$$Y_{n_2}^{\nu_2 *}(\omega_2) = (-1)^{\nu_2 - \nu_2} Y_{n_2}(\omega_2)$$

then

$$\sum_{l,\lambda} \tilde{E}_Y(m\ n\ l,k)C(m\ n\ l,\mu\ \nu\ \lambda)Y_l^{\lambda *} =$$

$$\frac{\rho}{4\pi}\Big\{ \sum \hat{E}_h(m\ n_1 l_1 k)C(n\ m_1 l_1 \mu\ \nu_1\lambda_1)Y_{l_1}^{\lambda_1 *} \sum \tilde{E}_f^*(n_1 n\ l_2,k)\cdot$$

$$C(n_1 n\ l_2,\nu_1 - \nu_1\ \lambda_2)(-1)^{\nu}Y_{l_2}^{\lambda_2}\ \Big\}$$

If we look at $Y_l^{\lambda}(\theta_k\phi_k)$, let $\theta_k = 0$, then $Y_l^{\lambda} \neq 0$ if $\lambda = 0$.

$$Y_l^0 = \left(\frac{2\ l+1}{4\pi}\right)^{\frac{1}{2}} \frac{1}{2^l l!} \left(\frac{d}{dx}\right)^l (x^2-1)^l$$

where $\frac{1}{2^l l!}\left(\frac{d}{dx}\right)^l (x-1)^l = 1$; for $l = 1,2,3,$

so

$$Y_1^o = \left(\frac{2\ 1+1}{4\pi}\right)^{\frac{1}{2}}$$

Then

$$Y_1^\lambda(\theta_k\phi_k) = Y_1^\lambda(0,\phi_k) = \left(\frac{2\ 1+1}{4}\right)^{\frac{1}{2}} \text{ when } \lambda = 0$$

$$\Sigma\ \tilde{E}_Y(m\ n\ 1,k)C(m\ n\ 1,\mu\ \nu\ o)\left(\frac{2\ 1+1}{4\pi}\right)^{\frac{1}{2}} = 4\pi\ \tilde{E}_Y(m\ n\ \mu\ k)$$

where $\tilde{E}_Y(mn\mu k)$ is in body-fixed coordinates.

$$4\pi\ \tilde{E}_Y(m\ n\ \mu\ k) = \frac{\rho}{4\pi}\ \sum_{\bar{m}}\ \tilde{E}_h(m\ n_1\ \mu\ k)\cdot$$

$$\{\tilde{E}_f(n_1 n\ \mu\ k)^*\ (-1)^\nu\}\ (4\pi)^2$$

or

$$\tilde{E}_Y(m\ n\ \mu\ k) = \rho\sum_{n}\ \tilde{E}_h(m\ n_1\ \mu\ k)\tilde{E}_f^*(n_1 n\ \nu\ k)\ (-1)^\nu$$

so

$$\tilde{E}_Y(1\ 1'm_1 k) = \rho\sum_{1''}\ \tilde{E}_h(1\ 1''\ mk(-1)^m\ E_f(1''\ 1'mk)$$

where

$$\tilde{E}_f(m\ n\ 1,k) = i^1(4\pi)\int_o^\infty dr\ r^2\ J_1(kr)E_f(m\ n\ 1,r)$$

$$\tilde{E}_f^*(m\ n\ 1,k) = (-1)^1\ i^1(4\pi)\ \int_o^\infty dr\ r^2\ J_1(kr)E_f^*(m\ n\ 1,r)$$

and

$$\tilde{E}_f^*(m\ n\ 1,k) = (-1)^1\ \ \tilde{E}_f(m\ n\ 1,k)$$

CHAPTER XIII

COMPARISON

In order to compare our results with previous work, we chose Dr. Haile's (18) since we have $E_Y(l_1 l_2 m\ r)$ and Dr. Haile's data are $E_g(l_1 l_2 m\ r)$, so we transferred our data as follows.

Since

$$\frac{Y(12)}{Y^o(r_{12})} - 1 = 4\pi \sum\sum E_Y(l\ l'\ m\ r) Y_l^m(\omega_1) Y_{l'}^{\bar{m}}(\omega_2) \qquad (12\text{-}1)$$

or

$$\frac{g(12) e^{-\beta u_a}}{g^o(r_{12})} - 1 = 4\pi \sum\sum E_Y(l\ l'm\ r) Y_l^m(\omega_1) Y_{l'}^{\bar{m}}(\omega_2) \qquad (12\text{-}2)$$

and

$$g(12) = g^o(r_{12})(4\pi \sum\sum E_Y(l\ l'm\ r) Y_l^m(\omega_1) Y_l^{\bar{m}}(\omega_2) e^{-\beta u_a} + g^o(r_{12}) e^{\beta u_a}$$

Expanding $e^{\beta u_a}$ in spherical harmonic, we have

$$g(12) = g^o(r_{12})(4\pi\Sigma\Sigma E_Y(l\ l'm\ r) Y_l^m Y_{l'}^{\bar{m}})(4\pi\Sigma\Sigma E_\mu(L\ L'M\ r) Y_L^M Y_{L'}^M) + g^o e^{\beta u_a}$$

Expand the left hand side

$$4\pi\Sigma\Sigma E_g(\lambda\lambda'\mu r) Y_\lambda^\mu Y_{\lambda'}^{\bar{\mu}} = \text{L.H.S.}$$

Multiply both sides by $Y_\Lambda^{k*} Y_{\Lambda'}^{k*}$ and integrate over $d\omega_1$ and $d\omega_2$ we have

$$E_g(\Lambda\ \Lambda'\ k\ r) = g^o(r)(4\pi)\sum_{\substack{L\\L'}}\sum_{M}\sum_{\substack{l\\l'}}\sum_{m} E_\mu(L\ L'M\ r)\cdot$$

$$E_Y(l\ l'm\ r)\int d\omega_1 \int d\omega_2\ Y_L^M(\omega_1)Y_{L'}^{\overline{M}}(\omega_2)Y_l^m(\omega_1)Y_{l'}^{\overline{m}}(\omega_2)\cdot$$

$$Y_\Lambda^{k*}(\omega_1)\ Y_{\Lambda'}^{k*}(\omega_2) + g^o E_\mu(\Lambda\ \Lambda^1\ k\ r)$$

$$E_g(\Lambda\ \Lambda'\ k\ r) = g^o(r)\sum_{\substack{L\\L'}}\sum_{M}\sum_{\substack{l\\l'}}\sum_{m} E_\mu(L\ L'\ M\ \Lambda)E_Y(l\ l'm\ r)\cdot$$

$$\left[\frac{(2L+1)\ (2L'+1)(2l'+1)(2l+1)}{(2\Lambda+1)\ \ (2\Lambda'+1)}\right]^{\frac{1}{2}}\ C(L\ l\Lambda\ ,\ M,m,k)\cdot$$

$$C(L\ l\ \Lambda,o\ o\ o)C(L'l'\Lambda',M'm'k)C(L'l'\Lambda',o\ o\ o)$$

$$+ g^o(r)\ E_\mu(\Lambda\ \Lambda'k\ r)$$

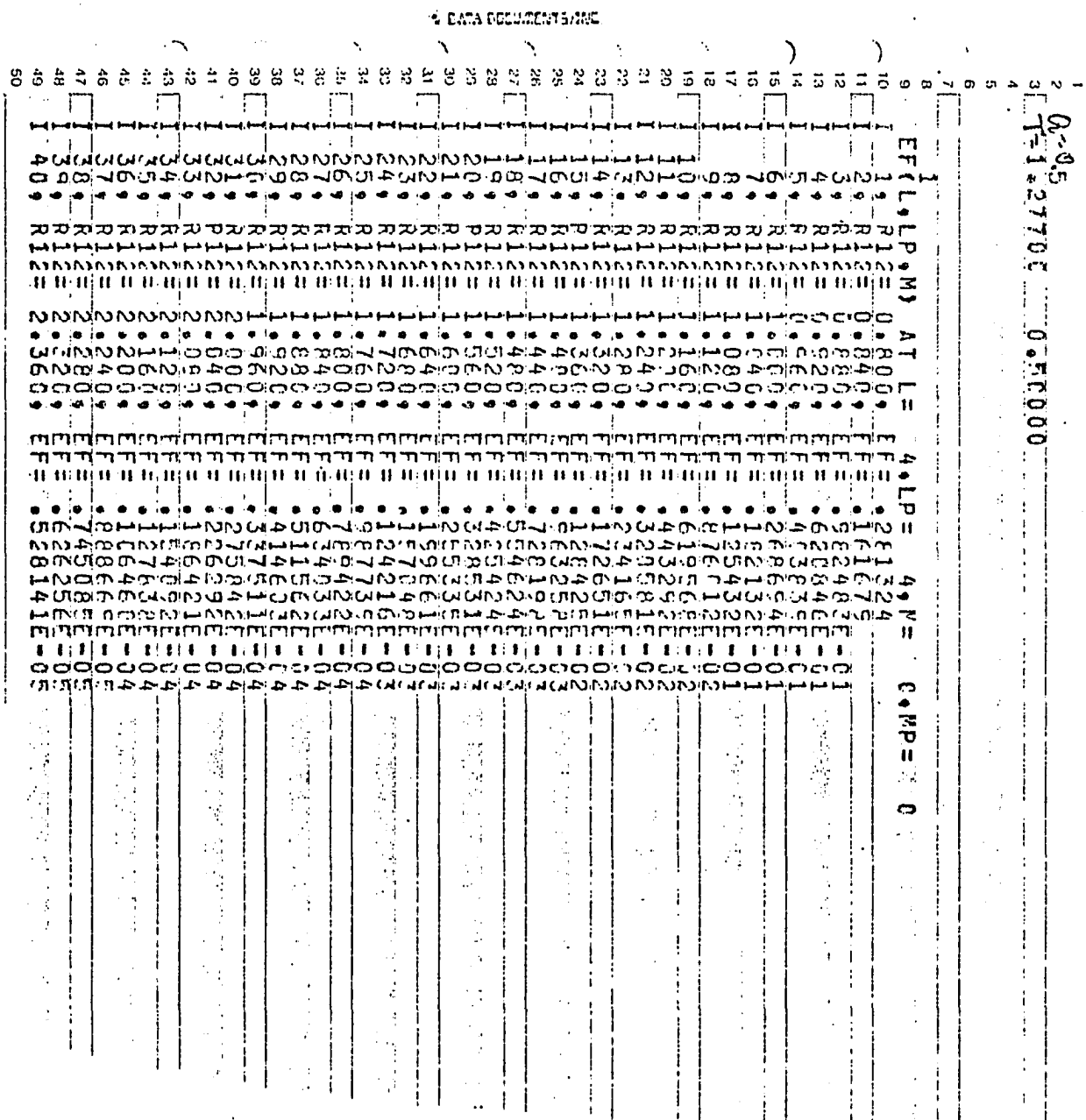
Here $E_\mu(l\ l'm\ r) = E_f(l\ l'm\ r)$

if $l\ l'm \neq o\ o\ o$

and if $l\ l'm = o\ o\ o$

$E_f(ooor) = E_\mu(ooor) - 1.$

In the coming pages we show our results for $E_f(\ell_1\ \ell_2\ m\ r)$, $E_Y(\ell_1\ \ell_2\ m\ r)$ and $E_g(\ell_1\ \ell_2\ m\ r)$ at different temperatures and quadrupole moments. Conclusions are given on page 150.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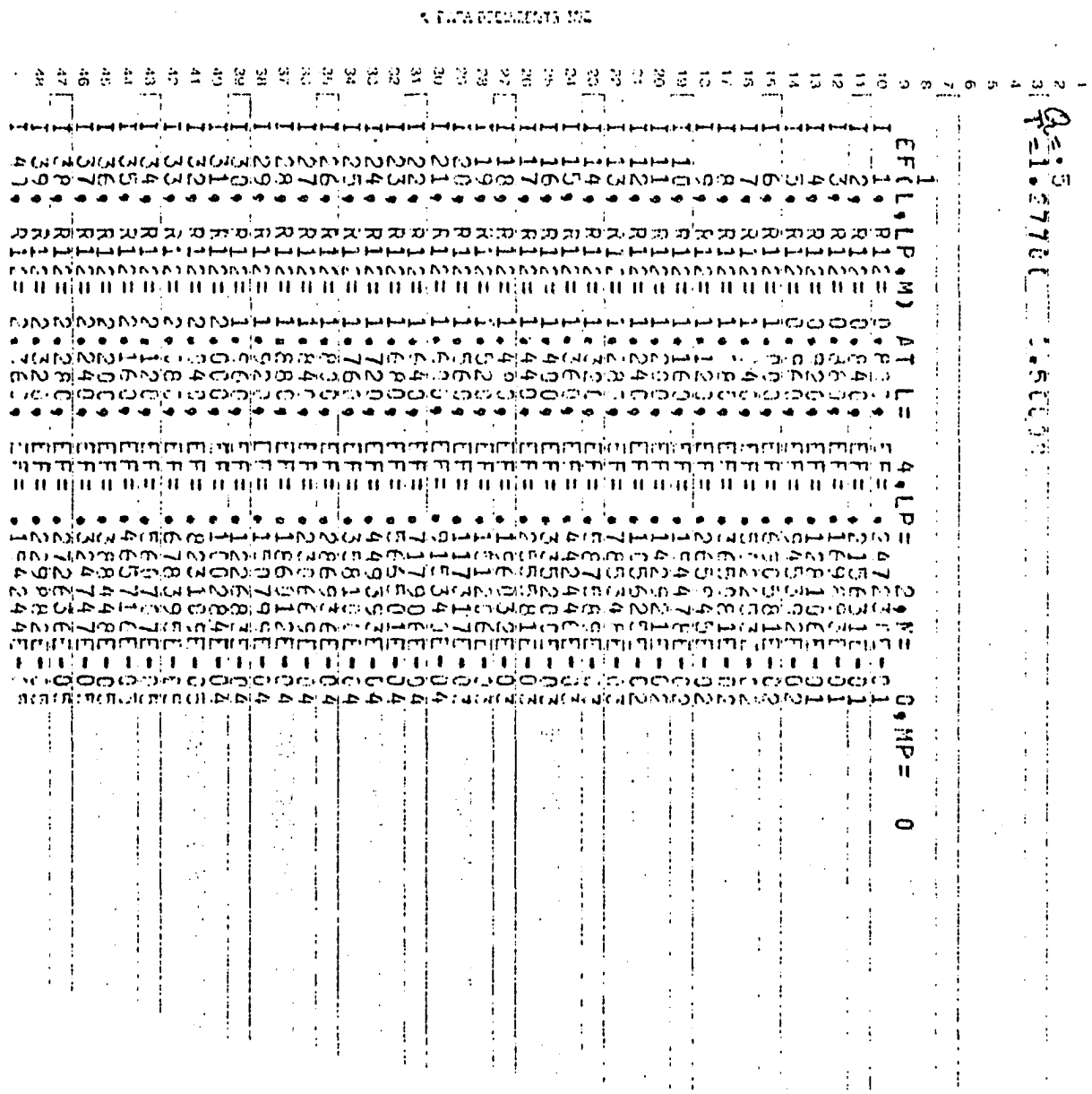
EF, L, LP, MP, AT L=
4, LP=
4, N=
3, MP=
0



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 I   2, R12= 0.840, EF=-.380092E-01
 I   3, R12= 0.880, EF=-.387324E-01
 I   4, R12= 0.920, EF=-.362775E-01
 I   5, R12= 0.960, EF=-.326569E-01
 I   6, R12= 1.000, EF=-.287892E-01
 I   7, R12= 1.040, EF=-.250904E-01
 I   8, R12= 1.080, EF=-.217329E-01
 I   9, R12= 1.120, EF=-.187696E-01
 I  10, R12= 1.160, EF=-.161966E-01
 I  11, R12= 1.200, EF=-.139814E-01
 I  12, R12= 1.240, EF=-.120855E-01
 I  13, R12= 1.280, EF=-.104664E-01
 I  14, R12= 1.320, EF=-.908481E-02
 I  15, R12= 1.360, EF=-.790579E-02
 I  16, R12= 1.400, EF=-.689724E-02
 I  17, R12= 1.440, EF=-.603405E-02
 I  18, R12= 1.480, EF=-.529345E-02
 I  19, R12= 1.520, EF=-.465645E-02
 I  20, R12= 1.560, EF=-.410719E-02
 I  21, R12= 1.600, EF=-.363238E-02
 I  22, R12= 1.640, EF=-.322082E-02
 I  23, R12= 1.680, EF=-.286313E-02
 I  24, R12= 1.720, EF=-.255146E-02
 I  25, R12= 1.760, EF=-.227918E-02
 I  26, R12= 1.800, EF=-.204065E-02
 I  27, R12= 1.840, EF=-.183117E-02
 I  28, R12= 1.880, EF=-.164678E-02
 I  29, R12= 1.920, EF=-.148406E-02
 I  30, R12= 1.960, EF=-.134014E-02
 I  31, R12= 2.000, EF=-.121254E-02
 I  32, R12= 2.040, EF=-.109917E-02
 I  33, R12= 2.080, EF=-.998220E-03
 I  34, R12= 2.120, EF=-.908143E-03
 I  35, R12= 2.160, EF=-.827613E-03
 I  36, R12= 2.200, EF=-.755465E-03
 I  37, R12= 2.240, EF=-.690713E-03
 I  38, R12= 2.280, EF=-.632485E-03
 I  39, R12= 2.320, EF=-.580039E-03
 I  40, R12= 2.360, EF=-.532712E-03
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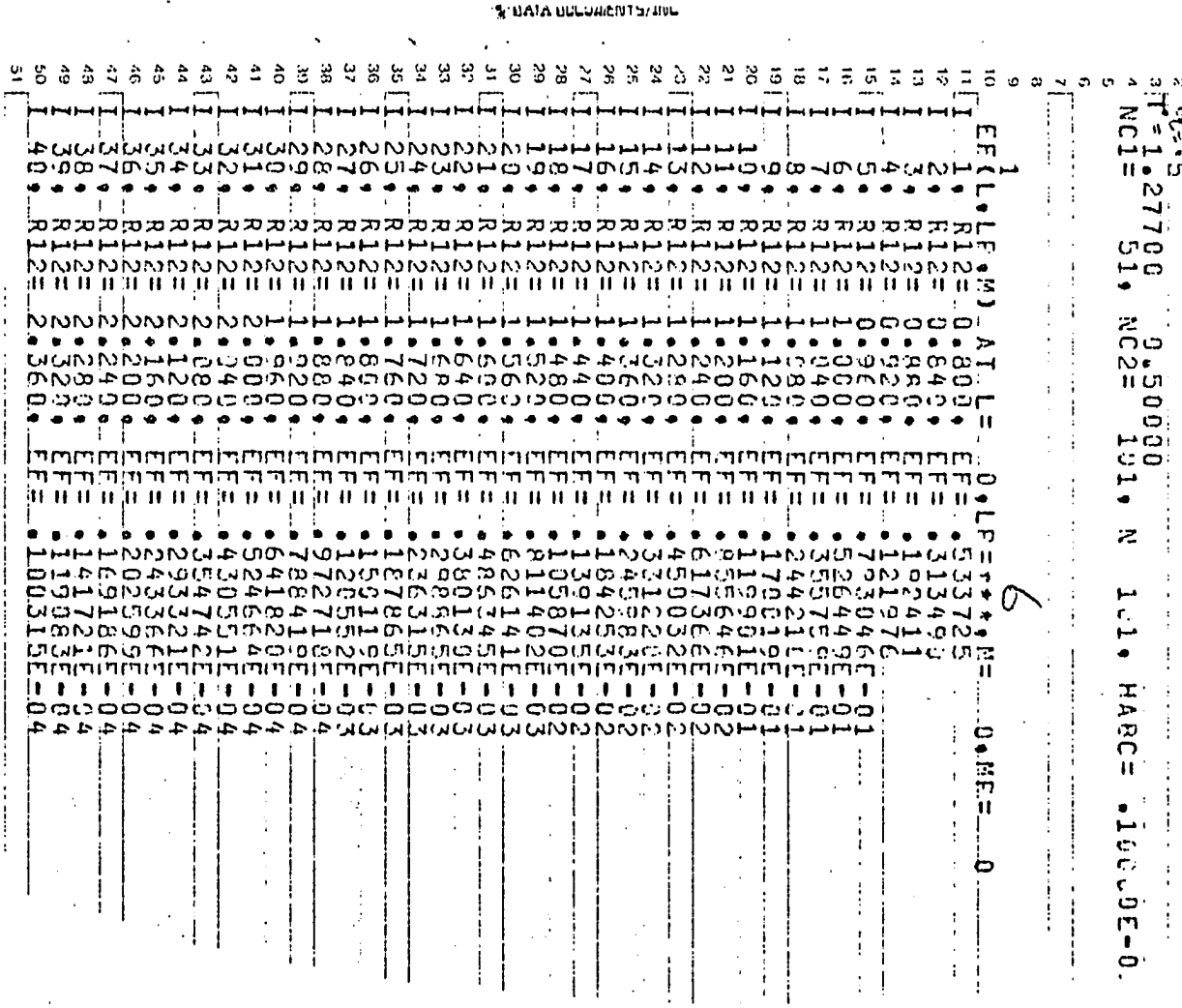
NC1= 51. NC2= 191. N 1.1. HARC= .100000E-0.
EF(L. LF. MJ AT L= 0. LP= 6. ME= 0. ME=

```
A=.5
T=1.27700   0.50000

 EF(L,LP,M) AT L=   6,LP=   2,M=   0,MP=  0
I   1, R12= 0.800, EF= .188276
I   2, R12= 0.840, EF= .114485
I   3, R12= 0.880, EF= .726426E-01
I   4, R12= 0.920, EF= .474375E-01
I   5, R12= 0.960, EF= .316405E-01
I   6, R12= 1.000, EF= .214613E-01
I   7, R12= 1.040, EF= .147656E-01
I   8, R12= 1.080, EF= .102886E-01
I   9, R12= 1.120, EF= .725254E-02
I  10, R12= 1.160, EF= .516723E-02
I  11, R12= 1.200, EF= .371902E-02
I  12, R12= 1.240, EF= .270247E-02
I  13, R12= 1.280, EF= .198181E-02
I  14, R12= 1.320, EF= .146588E-02
I  15, R12= 1.360, EF= .109328E-02
I  16, R12= 1.400, EF= .821862E-03
I  17, R12= 1.440, EF= .622412E-03
I  18, R12= 1.480, EF= .474722E-03
I  19, R12= 1.520, EF= .364537E-03
I  20, R12= 1.560, EF= .281679E-03
I  21, R12= 1.600, EF= .219098E-03
I  22, R12= 1.640, EF= .171422E-03
I  23, R12= 1.680, EF= .134923E-03
I  24, R12= 1.720, EF= .106755E-03
I  25, R12= 1.760, EF= .849257E-04
I  26, R12= 1.800, EF= .679164E-04
I  27, R12= 1.840, EF= .545760E-04
I  28, R12= 1.880, EF= .440811E-04
I  29, R12= 1.920, EF= .357532E-04
I  30, R12= 1.960, EF= .291330E-04
I  31, R12= 2.000, EF= .238277E-04
I  32, R12= 2.040, EF= .195626E-04
I  33, R12= 2.080, EF= .161246E-04
I  34, R12= 2.120, EF= .133392E-04
I  35, R12= 2.160, EF= .110755E-04
I  36, R12= 2.200, EF= .922671E-05
I  37, R12= 2.240, EF= .771426E-05
I  38, R12= 2.280, EF= .646726E-05
I  39, R12= 2.320, EF= .543840E-05
I  40, R12= 2.360, EF= .458657E-05
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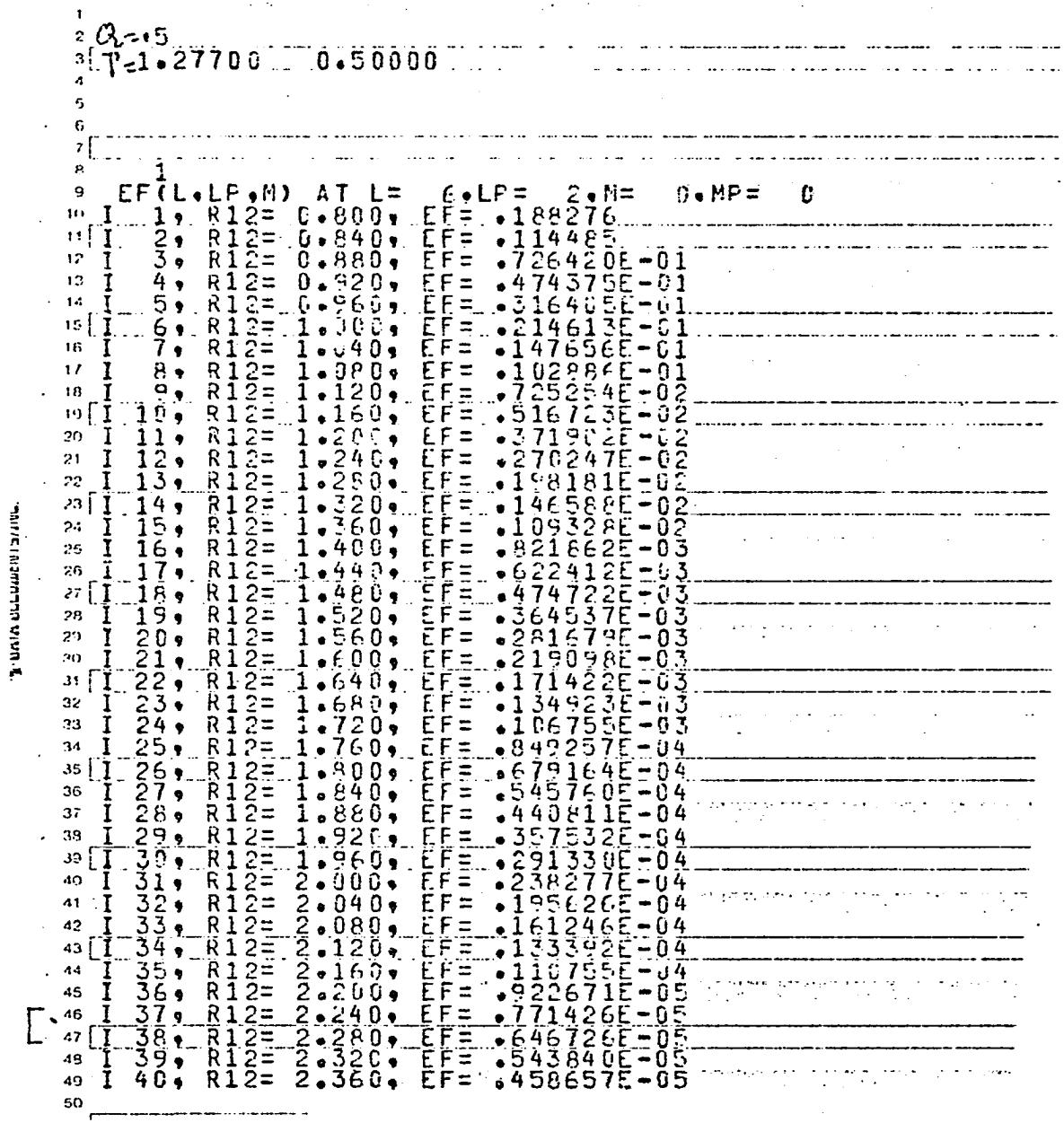
Q=.5
T=1.27700 0.50000
EF(L,LP,M) AT L= 6,LP= 2,M= 0,MP= 0
I 1, R12= 0.800, EF= .188276
I 2, R12= 0.840, EF= .114485
I 3, R12= 0.880, EF= .726420E-01
I 4, R12= 0.920, EF= .474375E-01
I 5, R12= 0.960, EF= .316405E-01
I 6, R12= 1.000, EF= .214613E-01
I 7, R12= 1.040, EF= .147656E-01
I 8, R12= 1.080, EF= .102884E-01
I 9, R12= 1.120, EF= .725254E-02
I 10, R12= 1.160, EF= .516723E-02
I 11, R12= 1.200, EF= .371902E-02
I 12, R12= 1.240, EF= .270247E-02
I 13, R12= 1.280, EF= .198181E-02
I 14, R12= 1.320, EF= .146588E-02
I 15, R12= 1.360, EF= .109328E-02
I 16, R12= 1.400, EF= .821662E-03
I 17, R12= 1.440, EF= .622412E-03
I 18, R12= 1.480, EF= .474722E-03
I 19, R12= 1.520, EF= .364537E-03
I 20, R12= 1.560, EF= .281679E-03
I 21, R12= 1.600, EF= .219098E-03
I 22, R12= 1.640, EF= .171422E-03
I 23, R12= 1.680, EF= .134923E-03
I 24, R12= 1.720, EF= .106755E-03
I 25, R12= 1.760, EF= .849257E-04
I 26, R12= 1.800, EF= .679164E-04
I 27, R12= 1.840, EF= .545760E-04
I 28, R12= 1.880, EF= .440811E-04
I 29, R12= 1.920, EF= .357532E-04
I 30, R12= 1.960, EF= .291330E-04
I 31, R12= 2.000, EF= .238277E-04
I 32, R12= 2.040, EF= .195626E-04
I 33, R12= 2.080, EF= .161246E-04
I 34, R12= 2.120, EF= .133392E-04
I 35, R12= 2.160, EF= .110755E-04
I 36, R12= 2.200, EF= .922671E-05
I 37, R12= 2.240, EF= .771426E-05
I 38, R12= 2.280, EF= .646726E-05
I 39, R12= 2.320, EF= .543840E-05
I 40, R12= 2.360, EF= .458657E-05

Ω = 1

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 NC1=    51,  NC2=   101,  N   101,  HARC=  .10000E-01  .10000E-01  .10000E-01

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I   2,  R12=  0.840,  EF=  15.6015
I   3,  R12=  0.880,  EF=  6.17115
I   4,  R12=  0.920,  EF=  2.97473
I   5,  R12=  0.960,  EF=  1.62934
I   6,  R12=  1.000,  EF=  .970972
I   7,  R12=  1.040,  EF=  .612864
I   8,  R12=  1.080,  EF=  .402888
I   9,  R12=  1.120,  EF=  .272914
I  10,  R12=  1.160,  EF=  .189177
I  11,  R12=  1.200,  EF=  .133567
I  12,  R12=  1.240,  EF=  .957502E-01
I  13,  R12=  1.280,  EF=  .695381E-01
I  14,  R12=  1.320,  EF=  .510791E-01
I  15,  R12=  1.360,  EF=  .379034E-01
I  16,  R12=  1.400,  EF=  .283868E-01
I  17,  R12=  1.440,  EF=  .214407E-01
I  18,  R12=  1.480,  EF=  .163222E-01
I  19,  R12=  1.520,  EF=  .125172E-01
I  20,  R12=  1.560,  EF=  .966587E-02
I  21,  R12=  1.600,  EF=  .751284E-02
I  22,  R12=  1.640,  EF=  .587592E-02
I  23,  R12=  1.680,  EF=  .462207E-02
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I  25,  R12=  1.760,  EF=  .290777E-02
I  26,  R12=  1.800,  EF=  .232425E-02
I  27,  R12=  1.840,  EF=  .186697E-02
I  28,  R12=  1.880,  EF=  .150666E-02
I  29,  R12=  1.920,  EF=  .122135E-02
I  30,  R12=  1.960,  EF=  .994328E-03
I  31,  R12=  2.000,  EF=  .812820E-03
I  32,  R12=  2.040,  EF=  .667090E-03
I  33,  R12=  2.080,  EF=  .549562E-03
I  34,  R12=  2.120,  EF=  .454456E-03
I  35,  R12=  2.160,  EF=  .377123E-03
I  36,  R12=  2.200,  EF=  .314002E-03
I  37,  R12=  2.240,  EF=  .262315E-03
I  38,  R12=  2.280,  EF=  .219851E-03
I  39,  R12=  2.320,  EF=  .184817E-03
I  40,  R12=  2.360,  EF=  .155831E-03
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ℓ = 1

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I   3,  R12=  0.880,  EF=-.316399
I   4,  R12=  0.920,  EF=-.736720E-01
I   5,  R12=  0.960,  EF=-.152476E-02
I   6,  R12=  1.000,  EF= .200856E-01
I   7,  R12=  1.040,  EF= .247531E-01
I   8,  R12=  1.080,  EF= .234871E-01
I   9,  R12=  1.120,  EF= .203224E-01
I  10,  R12=  1.160,  EF= .168272E-01
I  11,  R12=  1.200,  EF= .136010E-01
I  12,  R12=  1.240,  EF= .108397E-01
I  13,  R12=  1.280,  EF= .856861E-02
I  14,  R12=  1.320,  EF= .674204E-02
I  15,  R12=  1.360,  EF= .529343E-02
I  16,  R12=  1.400,  EF= .415326E-02
I  17,  R12=  1.440,  EF= .326118E-02
I  18,  R12=  1.480,  EF= .250487E-02
I  19,  R12=  1.520,  EF= .202190E-02
I  20,  R12=  1.560,  EF= .159840E-02
I  21,  R12=  1.600,  EF= .126752E-02
I  22,  R12=  1.640,  EF= .100255E-02
I  23,  R12=  1.680,  EF= .805315E-03
I  24,  R12=  1.720,  EF= .645386E-03
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I  26,  R12=  1.800,  EF= .419765E-03
I  27,  R12=  1.840,  EF= .339474E-03
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I  36,  R12=  2.200,  EF= .594884E-04
I  37,  R12=  2.240,  EF= .498377E-04
I  38,  R12=  2.280,  EF= .418453E-04
I  39,  R12=  2.320,  EF= .352374E-04
I  40,  R12=  2.360,  EF= .297567E-04
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ℓ2 = 1

```
T= 1.29400    1.00000
 NC1=    51, NC2=  101, N  101, HARC= .10000E-01 .10000E-01 .10000E-01

      1
  EF(L,LP,M) AT L=   2,LP=   2,M=  1,MP= -1
I   1,  R12=  0.800,  EF=-31.4360
I   2,  R12=  0.840,  EF=-9.56947
I   3,  R12=  0.880,  EF=-4.00874
I   4,  R12=  0.920,  EF=-2.09354
I   5,  R12=  0.960,  EF=-1.27314
I   6,  R12=  1.000,  EF=-.859938
I   7,  R12=  1.040,  EF=-.624479
I   8,  R12=  1.080,  EF=-.470931
I   9,  R12=  1.120,  EF=-.377118
I  10,  R12=  1.160,  EF=-.305818
I  11,  R12=  1.200,  EF=-.252561
I  12,  R12=  1.240,  EF=-.211441
I  13,  R12=  1.280,  EF=-.178885
I  14,  R12=  1.320,  EF=-.152611
I  15,  R12=  1.360,  EF=-.131092
I  16,  R12=  1.400,  EF=-.113260
I  17,  R12=  1.440,  EF=-.983466E-01
I  18,  R12=  1.480,  EF=-.857764E-01
I  19,  R12=  1.520,  EF=-.751130E-01
I  20,  R12=  1.560,  EF=-.660166E-01
I  21,  R12=  1.600,  EF=-.582181E-01
I  22,  R12=  1.640,  EF=-.515032E-01
I  23,  R12=  1.680,  EF=-.456985E-01
I  24,  R12=  1.720,  EF=-.406617E-01
I  25,  R12=  1.760,  EF=-.362763E-01
I  26,  R12=  1.800,  EF=-.324458E-01
I  27,  R12=  1.840,  EF=-.290896E-01
I  28,  R12=  1.880,  EF=-.261412E-01
I  29,  R12=  1.920,  EF=-.235434E-01
I  30,  R12=  1.960,  EF=-.212486E-01
I  31,  R12=  2.000,  EF=-.192169E-01
I  32,  R12=  2.040,  EF=-.174131E-01
I  33,  R12=  2.080,  EF=-.158085E-01
I  34,  R12=  2.120,  EF=-.143777E-01
I  35,  R12=  2.160,  EF=-.130993E-01
I  36,  R12=  2.200,  EF=-.119546E-01
I  37,  R12=  2.240,  EF=-.109277E-01
I  38,  R12=  2.280,  EF=-.100347E-01
I  39,  R12=  2.320,  EF=-.917359E-02
I  40,  R12=  2.360,  EF=-.842384E-02
```

T=1.29400E 00
KC1= 51. KC2= 101. N 101. HARC= .10000E-01 .10000E-01 .10000E-01
EF(L,LP,B) AT L= 4 LP= 4 N= 3 NP= -3

$\theta = 1$

T=1.25400 1.00000

NC1= 51, NC2= 151, N= 101, HABC= .10000E-01 .10000E-01 .10000E-01

1

EF(L,LP,M) AT L= 4,LP= 0,M= 0,MP= 0

I	1,	R12= 0.800,	EF=	26.8616
I	2,	R12= 0.840,	EF=	6.21228
I	3,	R12= 0.880,	EF=	2.00553
I	4,	R12= 0.920,	EF=	.816966
I	5,	R12= 0.960,	EF=	.392141
I	6,	R12= 1.000,	EF=	.211689
I	7,	R12= 1.040,	EF=	.124436
I	8,	R12= 1.080,	EF=	.778562E-01
I	9,	R12= 1.120,	EF=	.510185E-01
I	10,	R12= 1.160,	EF=	.346154E-01
I	11,	R12= 1.200,	EF=	.241187E-01
I	12,	R12= 1.240,	EF=	.171586E-01
I	13,	R12= 1.280,	EF=	.124128E-01
I	14,	R12= 1.320,	EF=	.915421E-02
I	15,	R12= 1.360,	EF=	.675589E-02
I	16,	R12= 1.400,	EF=	.506453E-02
I	17,	R12= 1.440,	EF=	.383090E-02
I	18,	R12= 1.480,	EF=	.292153E-02
I	19,	R12= 1.520,	EF=	.224461E-02
I	20,	R12= 1.560,	EF=	.173647E-02
I	21,	R12= 1.600,	EF=	.135206E-02
I	22,	R12= 1.640,	EF=	.105917E-02
I	23,	R12= 1.680,	EF=	.834541E-03
I	24,	R12= 1.720,	EF=	.661147E-03
I	25,	R12= 1.760,	EF=	.526536E-03
I	26,	R12= 1.800,	EF=	.421413E-03
I	27,	R12= 1.840,	EF=	.338908E-03
I	28,	R12= 1.880,	EF=	.273805E-03
I	29,	R12= 1.920,	EF=	.222157E-03
I	30,	R12= 1.960,	EF=	.180580E-03
I	31,	R12= 2.000,	EF=	.148030E-03
I	32,	R12= 2.040,	EF=	.121558E-03
I	33,	R12= 2.080,	EF=	.100194E-03
I	34,	R12= 2.120,	EF=	.828761E-04
I	35,	R12= 2.160,	EF=	.687935E-04
I	36,	R12= 2.200,	EF=	.572571E-04
I	37,	R12= 2.240,	EF=	.478706E-04
I	38,	R12= 2.280,	EF=	.401206E-04
I	39,	R12= 2.320,	EF=	.337278E-04
I	40,	R12= 2.360,	EF=	.284353E-04

T R=1

```
T=1.29400    1.00000
NC1=    51.  NC2=   101.  N   101.  HAEC=  .10000E-01  .10000E-01  .10000E-01

 1
EF(L,LP,M) AT L=   4,LP=   4,M=   0,MP=   0
I   1,  R12=  0.800,  EF=  48.4595
I   2,  R12=  0.840,  EF=  12.1474
I   3,  R12=  0.880,  EF=  4.23542
I   4,  R12=  0.920,  EF=  1.64893
I   5,  R12=  0.960,  EF=  .941577
I   6,  R12=  1.000,  EF=  .533412
I   7,  R12=  1.040,  EF=  .325597
I   8,  R12=  1.080,  EF=  .209592
I   9,  R12=  1.120,  EF=  .140235
I  10,  R12=  1.160,  EF=  .965767E-01
I  11,  R12=  1.200,  EF=  .680029E-01
I  12,  R12=  1.240,  EF=  .487334E-01
I  13,  R12=  1.280,  EF=  .354313E-01
I  14,  R12=  1.320,  EF=  .260755E-01
I  15,  R12=  1.360,  EF=  .193945E-01
I  16,  R12=  1.400,  EF=  .145609E-01
I  17,  R12=  1.440,  EF=  .110250E-01
I  18,  R12=  1.480,  EF=  .841277E-02
I  19,  R12=  1.520,  EF=  .646586E-02
I  20,  R12=  1.560,  EF=  .500312E-02
I  21,  R12=  1.600,  EF=  .389593E-02
I  22,  R12=  1.640,  EF=  .305203E-02
I  23,  R12=  1.680,  EF=  .240460E-02
I  24,  R12=  1.720,  EF=  .190483E-02
I  25,  R12=  1.760,  EF=  .151680E-02
I  26,  R12=  1.800,  EF=  .121381E-02
I  27,  R12=  1.840,  EF=  .975973E-03
I  28,  R12=  1.880,  EF=  .788311E-03
I  29,  R12=  1.920,  EF=  .639529E-03
I  30,  R12=  1.960,  EF=  .521009E-03
I  31,  R12=  2.000,  EF=  .426176E-03
I  32,  R12=  2.040,  EF=  .349961E-03
I  33,  R12=  2.080,  EF=  .288461E-03
I  34,  R12=  2.120,  EF=  .238625E-03
I  35,  R12=  2.160,  EF=  .198084E-03
I  36,  R12=  2.200,  EF=  .164590E-03
I  37,  R12=  2.240,  EF=  .137871E-03
I  38,  R12=  2.280,  EF=  .115567E-03
I  39,  R12=  2.320,  EF=  .971733E-04
I  40,  R12=  2.360,  EF=  .819412E-04
```

a = 1

T=1.25400 1.00000
NC1= 51, NC2= 101, N 101, HAPC= .10000E-01 .10000E-01 .10000E-01

1

EF(L,LP,M) AT L= 4,LP= 4,M= 2,MP= -2

I	1,	R12=	0.800,	EF= P.03899
I	2,	R12=	0.840,	EF= 2.54556
I	3,	R12=	0.880,	EF= 1.05841
I	4,	R12=	0.920,	EF= .59 9477
I	5,	R12=	0.960,	EF= .29 9697
I	6,	R12=	1.000,	EF= .19 4200
I	7,	R12=	1.040,	EF= .119671
I	8,	R12=	1.080,	EF= .80770 E-01
I	9,	R12=	1.120,	EF= .56 0164 E-01
I	10,	R12=	1.160,	EF= .39 6387 E-01
I	11,	R12=	1.200,	EF= .28 4924 E-01
I	12,	R12=	1.240,	EF= .20 7422 E-01
I	13,	R12=	1.280,	EF= .15 2641 E-01
I	14,	R12=	1.320,	EF= .11 3369 E-01
I	15,	R12=	1.360,	EF= .84 9559 E-02
I	16,	R12=	1.400,	EF= .64 1054 E-02
I	17,	R12=	1.440,	EF= .48 7980 E-02
I	18,	R12=	1.480,	EF= .37 3750 E-02
I	19,	R12=	1.520,	EF= .28 8120 E-02
I	20,	R12=	1.560,	EF= .22 3494 E-02
I	21,	R12=	1.600,	EF= .17 4389 E-02
I	22,	R12=	1.640,	EF= .13 6849 E-02
I	23,	R12=	1.680,	EF= .10 7972 E-02
I	24,	R12=	1.720,	EF= .85 6336 E-03
I	25,	R12=	1.760,	EF= .68 2 E-03
I	26,	R12=	1.800,	EF= .54 670 E-03
I	27,	R12=	1.840,	EF= .43 989 E-03
I	28,	R12=	1.880,	EF= .35 550 E-03
I	29,	R12=	1.920,	EF= .28 804 E-03
I	30,	R12=	1.960,	EF= .23 13 E-03
I	31,	R12=	2.000,	EF= .19 241 E-03
I	32,	R12=	2.040,	EF= .15 803 E-03
I	33,	R12=	2.080,	EF= .13 E-03
I	34,	R12=	2.120,	EF= .11 78 E-03
I	35,	R12=	2.160,	EF= .89 521 E-04
I	36,	R12=	2.200,	EF= .74 590 E-04
I	37,	R12=	2.240,	EF= .62 325 E-04
I	38,	R12=	2.280,	EF= .52 2 E-04
I	39,	R12=	2.320,	EF= .43 935 E-04
I	40,	R12=	2.360,	EF= .37 0 E-04

	0 0 0	2 0 2	4 0 4	2 2 0
0.8250	0.0000000E 00	0.0000000E 00	0.0000000E 00	0.0000000E 00
0.8500	0.1972410E 00	-0.7115501E-01	0.1383500E-01	-0.3529525E 01
0.8750	0.2100220E 00	-0.4575300E-01	0.1072000E-01	-0.3668221E 01
0.9000	0.2295690E 00	-0.1993400E-01	0.7521000E-02	-0.3649111E 01
0.9250	0.2543350E 00	0.5332999E-02	0.4260998E-02	-0.3579915E 01
0.9500	0.2927770E 00	0.2873400E-01	0.9699999E-03	-0.3469764E 01
0.9750	0.3134880E 00	0.4911300E-01	-0.2319000E-02	-0.3322549E 01
1.0000	0.3452580E 00	0.6553698E-01	-0.5564999E-02	-0.3146010E 01
1.0250	0.3770340E 00	0.7746798E-01	-0.8731999E-02	-0.2941830E 01
1.0500	0.4078280E 00	0.8481902E-01	-0.1178600E-01	-0.2711453E 01
1.0750	0.4366330E 00	0.8792198E-01	-0.1470300E-01	-0.2455327E 01
1.1000	0.4624230E 00	0.8742702E-01	-0.1746100E-01	-0.2179078E 01
1.1250	0.4842520E 00	0.8415600E-01	-0.2004000E-01	-0.1883965E 01
1.1500	0.5013700E 00	0.7899398E-01	-0.2241100E-01	-0.1576423E 01
1.1750	0.5133070E 00	0.7280201E-01	-0.2454400E-01	-0.1262179E 01
1.2000	0.5199000E 00	0.6642503E-01	-0.2640300E-01	-0.9465950E 00
1.2250	0.5212920E 00	0.6064400E-01	-0.2795200E-01	-0.6343730E 00
1.2500	0.5179310E 00	0.5604900E-01	-0.2915700E-01	-0.3294910E 00
1.2750	0.5105550E 00	0.5286500E-01	-0.2998600E-01	-0.3541500E-01
1.3000	0.5001190E 00	0.5084200E-01	-0.3041100E-01	0.2443640E 00
1.3250	0.4877080E 00	0.4934100E-01	-0.3041000E-01	0.5058770E 00
1.3500	0.4744480E 00	0.4759900E-01	-0.2998200E-01	0.7447900E 00
1.3750	0.4614100E 00	0.4504300E-01	-0.2914800E-01	0.9569720E 00
1.4000	0.4494560E 00	0.4146700E-01	-0.2796000E-01	0.1138954E 01
1.4250	0.4390520E 00	0.3701900E-01	-0.2649300E-01	0.1287997E 01
1.4500	0.4301680E 00	0.3204900E-01	-0.2483300E-01	0.1402000E 01
1.4750	0.4223800E 00	0.2694000E-01	-0.2306400E-01	0.1479455E 01
1.5000	0.4151780E 00	0.2201200E-01	-0.2124800E-01	0.1519379E 01
1.5250	0.4082410E 00	0.1748000E-01	-0.1942400E-01	0.1521185E 01
1.5500	0.4015040E 00	0.1344500E-01	-0.1760800E-01	0.1484695E 01
1.5750	0.3950000E 00	0.9904999E-02	-0.1580300E-01	0.1410361E 01
1.6000	0.3887020E 00	0.6795000E-02	-0.1400400E-01	0.1299505E 01
1.6250	0.3825230E 00	0.4041001E-02	-0.1221100E-01	0.1154409E 01
1.6500	0.3764370E 00	0.1610000E-02	-0.1043000E-01	0.9783370E 00
1.6750	0.3705200E 00	-0.4930000E-03	-0.8671999E-02	0.7756160E 00
1.7000	0.3648300E 00	-0.2271000E-02	-0.6955002E-02	0.5517200E 00
1.7250	0.3593090E 00	-0.3763000E-02	-0.5295001E-02	0.3133340E 00

1.7500	0.3539320E 00	-0.5004998E-02	-0.3689000E-02	0.6849700E-01
1.7750	0.3491050E 00	-0.5947001E-02	-0.2105000E-02	-0.1731990E 00
1.8000	0.3459860E 00	-0.6383002E-02	-0.4560001E-03	-0.4005750E 00
1.8250	0.3463810E 00	-0.5952001E-02	0.1349000E-02	-0.6009770E 00
1.8500	0.3521200E 00	-0.4246999E-02	0.3473000E-02	-0.7604560E 00
1.8750	0.3641900E 00	-0.9630001E-03	0.6014999E-02	-0.8645900E 00
1.9000	0.3820410E 00	0.3954999E-02	0.9004001E-02	-0.9010270E 00
1.9250	0.4033070E 00	0.1021400E-01	0.1235100E-01	-0.8637910E 00
1.9500	0.4240510E 00	0.1716700E-01	0.1584500E-01	-0.7572770E 00
1.9750	0.4394470E 00	0.2389700E-01	0.1918300E-01	-0.5973450E 00
2.0000	0.4448010E 00	0.2942000E-01	0.2203900E-01	-0.4086820E 00
2.0250	0.4366710E 00	0.3294100E-01	0.2409700E-01	-0.2195930E 00
2.0500	0.4137130E 00	0.3407200E-01	0.2520000E-01	-0.5571500E-01
2.0750	0.3769270E 00	0.3289900E-01	0.2528500E-01	0.6607002E-01
2.1000	0.3292180E 00	0.2986700E-01	0.2442300E-01	0.1414450E 00
2.1250	0.2745290E 00	0.2556500E-01	0.2277200E-01	0.1777470E 00
2.1500	0.2169400E 00	0.2052600E-01	0.2053200E-01	0.1883060E 00
2.1750	0.1600470E 00	0.1514800E-01	0.1790600E-01	0.1855500E 00
2.2000	0.1066670E 00	0.9732001E-02	0.1507200E-01	0.1777930E 00
2.2250	0.5877400E-01	0.4551001E-02	0.1217100E-01	0.1689570E 00
2.2500	0.1756000E-01	-0.1210000E-03	0.9314001E-02	0.1588450E 00
2.2750	-0.1644100E-01	-0.4048001E-02	0.6579999E-02	0.1487830E 00
2.3000	-0.4317200E-01	-0.7102000E-02	0.4021998E-02	0.1373150E 00
2.3250	-0.6288803E-01	-0.9316999E-02	0.1674000E-02	0.1235550E 00
2.3500	-0.7603699E-01	-0.1087700E-01	-0.4469999E-03	0.1075310E 00
2.3750	-0.8321100E-01	-0.1206300E-01	-0.2332000E-02	0.9022200E-01
2.4000	0.0000000E 00	0.0000000E 00	0.0000000E 00	0.0000000E 00

sP.F

$E_f(R, R_l(r))$

$Q = 0.5$

$T = 1.277$

	ℓ_1^2 ℓ_2^2	ℓ_1^2 ℓ_2^4	ℓ_1^4 ℓ_2^2	ℓ_1^4 ℓ_2^4
0.8250	0.0000000E 00	0.0000000E 00	0.0000000E 00	0.0000000E 00
0.8500	0.2223957E 01	0.5995670E 00	-0.1441600E-01	-0.5277000E-02
0.8750	0.1467799E 01	0.5931160E 00	-0.1316700E-01	-0.5681001E-02
0.9000	0.1708579E 01	0.5852220E 00	-0.1174000E-01	-0.6046999E-02
0.9250	0.1548337E 01	0.5757110E 00	-0.1015800E-01	-0.6377999E-02
0.9500	0.1389102E 01	0.5629000E 00	-0.8453000E-02	-0.6673001E-02
0.9750	0.1232281E 01	0.5477440E 00	-0.6664999E-02	-0.6925999E-02
1.0000	0.1078580E 01	0.5311580E 00	-0.4843999E-02	-0.7126000E-02
1.0250	0.9272130E 00	0.5137960E 00	-0.3036000E-02	-0.7268000E-02
1.0500	0.7783810E 00	0.4971510E 00	-0.1284000E-02	-0.7344000E-02
1.0750	0.6316130E 00	0.4808410E 00	0.3770001E-03	-0.7353000E-02
1.1000	0.4880890E 00	0.4645520E 00	0.1922000E-02	-0.7295001E-02
1.1250	0.3483780E 00	0.4491110E 00	0.3370000E-02	-0.7173000E-02
1.1500	0.2140470E 00	0.4339670E 00	0.4584000E-02	-0.6987002E-02
1.1750	0.9628899E-01	0.4191980E 00	0.5667001E-02	-0.6737001E-02
1.2000	-0.3401800E-01	0.4053240E 00	0.6560002E-02	-0.6423000E-02
1.2250	-0.1462410E 00	0.3925280E 00	0.7249001E-02	-0.6044000E-02
1.2500	-0.2498920E 00	0.3807520E 00	0.7718001E-02	-0.5600002E-02
1.2750	-0.3444550E 00	0.3699550E 00	0.7961001E-02	-0.5098000E-02
1.3000	-0.4291750E 00	0.3597990E 00	0.7973999E-02	-0.4542999E-02
1.3250	-0.5028560E 00	0.3497960E 00	0.7764999E-02	-0.3947999E-02
1.3500	-0.5647320E 00	0.3398200E 00	0.7346001E-02	-0.3324000E-02
1.3750	-0.6135160E 00	0.3094920E 00	0.6737001E-02	-0.2686000E-02
1.4000	-0.6488280E 00	0.2864190E 00	0.5961999E-02	-0.2048000E-02
1.4250	-0.6704540E 00	0.2611570E 00	0.5050000E-02	-0.1424000E-02
1.4500	-0.6783860E 00	0.2330510E 00	0.4032999E-02	-0.8250000E-03
1.4750	-0.6720770E 00	0.2031810E 00	0.2945000E-02	-0.2619999E-03
1.5000	-0.6540660E 00	0.1722310E 00	0.1819000E-02	0.2580001E-03
1.5250	-0.6226020E 00	0.1406960E 00	0.6839999E-03	0.7269999E-03
1.5500	-0.5789190E 00	0.1088650E 00	-0.3930000E-03	0.1138000E-02
1.5750	-0.5236920E 00	0.7694000E-01	-0.1405000E-02	0.1485000E-02
1.6000	-0.4578660E 00	0.4542300E-01	-0.2304000E-02	0.1759000E-02
1.6250	-0.3826490E 00	0.1446600E-01	-0.3057000E-02	0.1954000E-02
1.6500	-0.2995130E 00	-0.1547600E-01	-0.3633000E-02	0.2063000E-02
1.6750	-0.2102610E 00	-0.4394500E-01	-0.4011001E-02	0.2084000E-02
1.7000	-0.1170770E 00	-0.7046199E-01	-0.4174002E-02	0.2017000E-02
1.7250	-0.2250100E-01	-0.9436801E-01	-0.4115999E-02	0.1866000E-02

S.f

$E_f(\ell_1 \ell_2 \ell_3 r)$

$Q = .5$

$T = 1.277$

1.7500	0.7054901E-01	-0.1151730E 00	-0.3840000E-02	0.1640000E-02
1.7750	0.1586780E 00	-0.1321600E 00	-0.3364000E-02	0.1354000E-02
1.8000	0.2371330E 00	-0.1443920E 00	-0.2719000E-02	0.1024000E-02
1.8250	0.3236460E 00	-0.1506630E 00	-0.1952000E-02	0.6740000E-03
1.8500	0.3515640E 00	-0.1497650E 00	-0.1126000E-02	0.3269999E-03
1.8750	0.3762320E 00	-0.1407200E 00	-0.3159000E-03	0.9000000E-05
1.9000	0.3739970E 00	-0.1230610E 00	0.4070001E-03	-0.2550001E-03
1.9250	0.3436670E 00	-0.9726599E-01	0.9730000E-03	-0.4480999E-03
1.9500	0.2661830E 00	-0.6529802E-01	0.1342000E-02	-0.5640001E-03
1.9750	0.2146270E 00	-0.3823750E-01	0.1501000E-02	-0.6019999E-03
2.0000	0.1339190E 00	0.4135000E-02	0.1466000E-02	-0.5750000E-03
2.0250	0.5659900E-01	0.3452000E-01	0.1092000E-02	-0.5040001E-03
2.0500	-0.1587700E-02	0.5727100E-01	0.1031000E-02	-0.4110000E-03
2.0750	-0.5289900E-01	0.7156101E-01	0.7460001E-03	-0.3130001E-03
2.1000	-0.7666800E-01	0.7716003E-01	0.4846000E-03	-0.2250000E-03
2.1250	-0.8466800E-01	0.7556999E-01	0.2720000E-03	-0.1530000E-03
2.1500	-0.8873300E-01	0.6897098E-01	0.1190000E-03	-0.9600000E-04
2.1750	-0.8388799E-01	0.5943300E-01	0.1400000E-04	-0.5000000E-04
2.2000	-0.7717001E-01	0.4853800E-01	-0.5300000E-04	-0.1400000E-04
2.2250	-0.6991899E-01	0.3754100E-01	-0.9800000E-04	0.1600000E-04
2.2500	-0.6263602E-01	0.2756600E-01	-0.1250000E-03	0.3700001E-04
2.2750	-0.5540500E-01	0.1942400E-01	-0.1430000E-03	0.4899999E-04
2.3000	-0.4803300E-01	0.1275000E-01	-0.1470000E-03	0.5300000E-04
2.3250	-0.4033600E-01	0.7220001E-02	-0.1410000E-03	0.5300000E-04
2.3500	-0.3243700E-01	0.2431000E-02	-0.1280000E-03	0.5300000E-04
2.3750	-0.2473800E-01	-0.1801900E-02	-0.1140000E-03	0.5700000E-04
2.4000	0.0000000E 00	0.0000000E 00	0.0000000E 00	0.0000000E 00

	4 2 6	4 4 0	4 4 2	4 4 4
0.8250	0.0000000E 00	0.0000000E 00	0.0000000E 00	0.0000000E 00
0.8500	-0.1034000E-02	0.3490000E-02	-0.1898000E-02	0.5190001E-03
0.8750	-0.1160000E-02	0.3424000E-02	-0.1660000E-02	0.3650000E-03
0.9000	-0.1252000E-02	0.3201000E-02	-0.1409000E-02	0.1620000E-03
0.9250	-0.1312000E-02	0.2863000E-02	-0.1137000E-02	0.6000000E-05
0.9500	-0.1350000E-02	0.2435000E-02	-0.8630001E-03	-0.1080000E-03
0.9750	-0.1380000E-02	0.1934000E-02	-0.5930001E-03	-0.1850000E-03
1.0000	-0.1415000E-02	0.1379000E-02	-0.3340000E-03	-0.2310000E-03
1.0250	-0.1462000E-02	0.8000000E-03	-0.9600000E-04	-0.2460000E-03
1.0500	-0.1523000E-02	0.2370000E-03	0.1050000E-03	-0.2310000E-03
1.0750	-0.1597000E-02	-0.2649999E-03	0.2560001E-03	-0.1870000E-03
1.1000	-0.1679000E-02	-0.6539999E-03	0.3460001E-03	-0.1170000E-03
1.1250	-0.1768000E-02	-0.9300001E-03	0.3700000E-03	-0.2700000E-04
1.1500	-0.1863000E-02	-0.1052000E-02	0.3320000E-03	0.6999999E-04
1.1750	-0.1967000E-02	-0.1037000E-02	0.2440000E-03	0.1630000E-03
1.2000	-0.2080000E-02	-0.9079999E-03	0.1230000E-03	0.2370000E-03
1.2250	-0.2200000E-02	-0.6970000E-03	-0.1100000E-04	0.2800000E-03
1.2500	-0.2322000E-02	-0.4410001E-03	-0.1390000E-03	0.2850001E-03
1.2750	-0.2439000E-02	-0.1740000E-03	-0.2440000E-03	0.2500000E-03
1.3000	-0.2540000E-02	0.7300000E-04	-0.3160001E-03	0.1780000E-03
1.3250	-0.2620000E-02	0.2800000E-03	-0.3500001E-03	0.7800000E-04
1.3500	-0.2677000E-02	0.4320000E-03	-0.3480001E-03	-0.3600000E-04
1.3750	-0.2719000E-02	0.5230000E-03	-0.3150001E-03	-0.1520000E-03
1.4000	-0.2726000E-02	0.5530000E-03	-0.2570001E-03	-0.2590001E-03
1.4250	-0.2732000E-02	0.5260000E-03	-0.1810000E-03	-0.3500001E-03
1.4500	-0.2733000E-02	0.4530000E-03	-0.9500000E-04	-0.4189999E-03
1.4750	-0.2733000E-02	0.3460001E-03	-0.6000000E-05	-0.4640000E-03
1.5000	-0.2735000E-02	0.2230000E-03	0.7800000E-04	-0.4850000E-03
1.5250	-0.2733000E-02	0.1000000E-03	0.1490000E-03	-0.4779999E-03
1.5500	-0.2723000E-02	-0.4000000E-05	0.1980000E-03	-0.4430001E-03
1.5750	-0.2698000E-02	-0.7600000E-04	0.2200000E-03	-0.3790001E-03
1.6000	-0.2650000E-02	-0.1090000E-03	0.2110000E-03	-0.2870001E-03
1.6250	-0.2575000E-02	-0.1010000E-03	0.1740000E-03	-0.1770000E-03
1.6500	-0.2471000E-02	-0.6100000E-04	0.1170000E-03	-0.6900001E-04
1.6750	-0.2338000E-02	-0.7000000E-05	0.5300000E-04	0.4899999E-04
1.7000	-0.2181000E-02	0.4200000E-04	-0.4000000E-05	0.1340000E-03
1.7250	-0.2006000E-02	0.6400001E-04	-0.4000000E-04	0.1820000E-03
1.7500	-0.1818000E-02	0.4200000E-04	-0.4499999E-04	0.1890000E-03
1.7750	-0.1623000E-02	-0.3500000E-04	-0.1500000E-04	0.1570000E-03
1.8000	-0.1426000E-02	-0.1680000E-03	0.4499999E-04	0.9400000E-04
1.8250	-0.1233000E-02	-0.3460001E-03	0.1290000E-03	0.1600001E-04
1.8500	-0.1052000E-02	-0.5480000E-03	0.2210000E-03	-0.6300000E-04
1.8750	-0.8910000E-03	-0.7460001E-03	0.3080000E-03	-0.1290000E-03
1.9000	-0.7610000E-03	-0.9059999E-03	0.3720000E-03	-0.1720000E-03
1.9250	-0.6700000E-03	-0.9979999E-03	0.4020000E-03	-0.1840000E-03
1.9500	-0.6220001E-03	-0.9989999E-03	0.3869999E-03	-0.1650000E-03
1.9750	-0.6150000E-03	-0.8980001E-03	0.3269999E-03	-0.1160000E-03
2.0000	-0.6400000E-03	-0.7250000E-03	0.2260000E-03	-0.4600000E-04
2.0250	-0.6850001E-03	-0.4439999E-03	0.9800000E-04	0.3600000E-04
2.0500	-0.7330000E-03	-0.1520000E-03	-0.3900001E-04	0.1160000E-03
2.0750	-0.7700000E-03	0.1280000E-03	-0.1650000E-03	0.1820000E-03
2.1000	-0.7890000E-03	0.3620000E-03	-0.2629999E-03	0.2250000E-03
2.1250	-0.7849999E-03	0.5270001E-03	-0.3229999E-03	0.2390000E-03
2.1500	-0.7620000E-03	0.6190001E-03	-0.3440001E-03	0.2270000E-03
2.1750	-0.7249999E-03	0.6510001E-03	-0.3350000E-03	0.1960000E-03
2.2000	-0.6830001E-03	0.6450000E-03	-0.3080000E-03	0.1570000E-03
2.2250	-0.6400000E-03	0.6210001E-03	-0.2770000E-03	0.1190000E-03
2.2500	-0.5999999E-03	0.5930001E-03	-0.2490000E-03	0.9700000E-04
2.2750	-0.5650001E-03	0.5640001E-03	-0.2260000E-03	0.7100000E-04
2.3000	-0.5320001E-03	0.5220000E-03	-0.2030000E-03	0.5000001E-04
2.3250	-0.5010001E-03	0.4550000E-03	-0.1720000E-03	0.4400000E-04
2.3500	-0.4670001E-03	0.3510001E-03	-0.1260000E-03	0.2399999E-04
2.3750	-0.4250000E-03	0.2290000E-03	-0.6500000E-04	-0.6000000E-05
2.4000	0.0000000E 00	0.0000000E 00	0.0000000E 00	0.0000000E 00

S.f

$E_s(l,l,l\,1)$

$Q = 0.5$

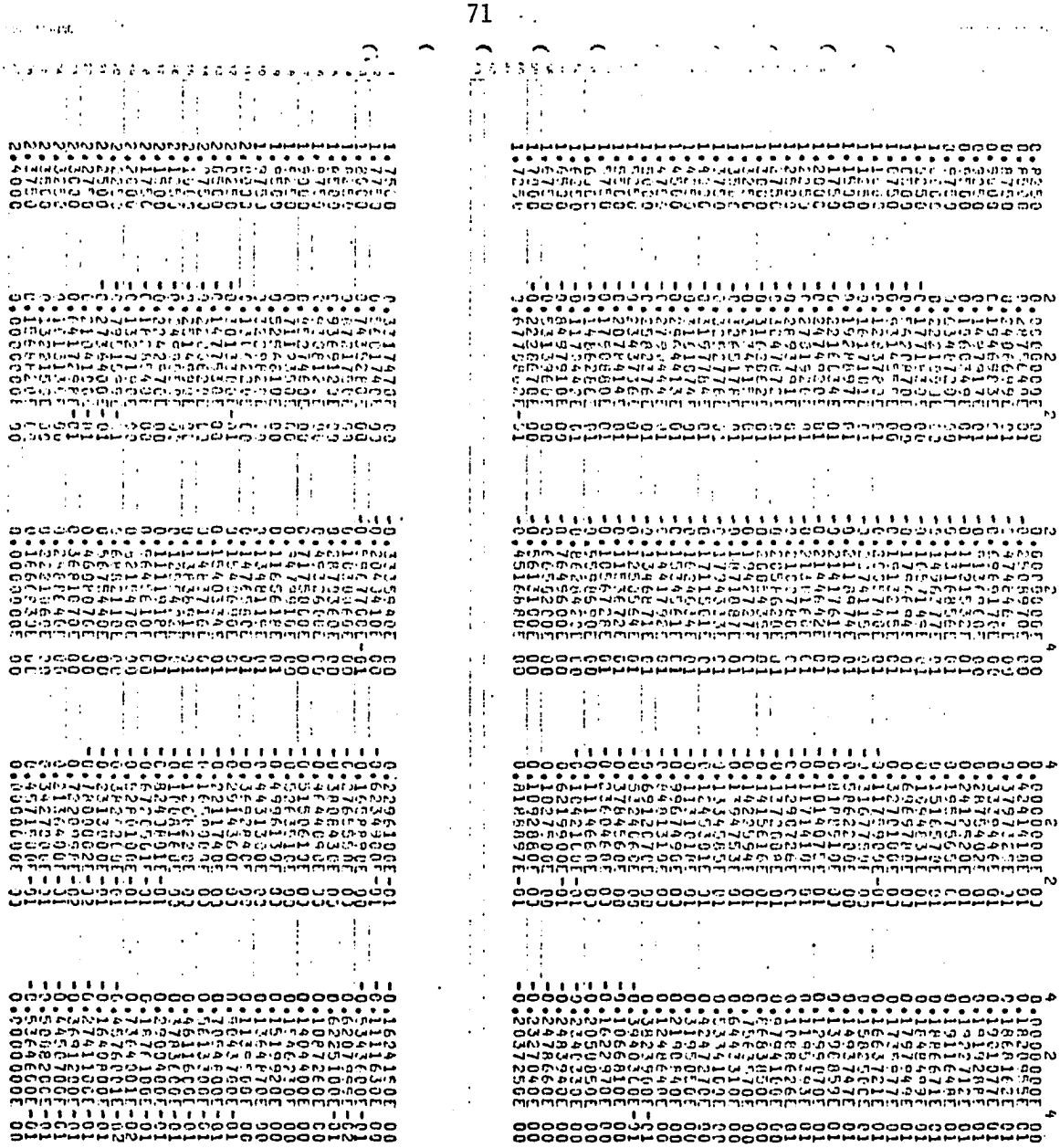
$T = 1.277$

space fixed

$E_f(\rho, \rho_c, r)$

$\alpha = 1$

$T = 1.29\,\mathrm{K}$


SP fixed coupling
$E_f(\ell, \beta_2, \beta_4)$
$\alpha = 1$
$T = 1.294$

S_f
$E_f(\rho, \rho_2, r)$
$Q=1$
$T=1.494$

BF
E f (l, l, r)
α = 1
T = 1.294

BC
$E_f(l, l_2, \omega)$
$a = 1$
$T = 1.294$

s.F $E_1(\ell_1 \ell_2 \ell\ r)$ Q=1 T=1.294 $E_F(\ell_1 \ell_2 \ell r)$ s.F Q=0.5 T=1.277

	4 4 6	4 4 8	4 4 6	4 4 8
0.8250	0.0000000E 00	0.0000000E 00	0.0000000E 00	0.0000000E 00
0.8500	0.1133500E-01	0.2416700E-01	0.6830001E-03	0.8999999E-04
0.8750	0.9544398E-02	0.2489200E-01	0.5800000E-03	0.1140000E-03
0.9000	0.7748000E-02	0.2598900E-01	0.4640000E-03	0.1400000E-03
0.9250	0.5924001E-02	0.2743000E-01	0.3430001E-03	0.1640000E-03
0.9500	0.4039999E-02	0.2909400E-01	0.2240000E-03	0.1820000E-03
0.9750	0.2097000E-02	0.3077900E-01	0.1130000E-03	0.1880000E-03
1.0000	0.1360000E-03	0.3227400E-01	0.1400000E-04	0.1770000E-03
1.0250	-0.1830000E-02	0.3345500E-01	-0.7200000E-04	0.1460000E-03
1.0500	-0.3865000E-02	0.3432600E-01	-0.1410000E-03	0.9299999E-04
1.0750	-0.6060001E-02	0.3495000E-01	-0.1920000E-03	0.1900000E-04
1.1000	-0.8448001E-02	0.3535100E-01	-0.2230000E-03	-0.6999999E-04
1.1250	-0.1094500E-01	0.3546400E-01	-0.2300000E-03	-0.1670000E-03
1.1500	-0.1338400E-01	0.3529500E-01	-0.2120000E-03	-0.2659999E-03
1.1750	-0.1556300E-01	0.3478200E-01	-0.1660000E-03	-0.3589999E-03
1.2000	-0.1725700E-01	0.3400700E-01	-0.9099999E-04	-0.4420001E-03
1.2250	-0.1822600E-01	0.3307000E-01	0.1200000E-04	-0.5089999E-03
1.2500	-0.1825300E-01	0.3208500E-01	0.1360000E-03	-0.5560000E-03
1.2750	-0.1720500E-01	0.3116400E-01	0.2720000E-03	-0.5760000E-03
1.3000	-0.1505800E-01	0.3038400E-01	0.4080001E-03	-0.5630001E-03
1.3250	-0.1166200E-01	0.2975400E-01	0.5270001E-03	-0.5129999E-03
1.3500	-0.7709000E-02	0.2922200E-01	0.6170000E-03	-0.4250000E-03
1.3750	-0.2731000E-02	0.2876700E-01	0.6670000E-03	-0.3060000E-03
1.4000	0.2884000E-02	0.2843700E-01	0.6740000E-03	-0.1670000E-03
1.4250	0.8914001E-02	0.2821800E-01	0.6420000E-03	-0.2300000E-04
1.4500	0.1514600E-01	0.2812100E-01	0.5760000E-03	0.1110000E-03
1.4750	0.2139000E-01	0.2809400E-01	0.4850000E-03	0.2250000E-03
1.5000	0.2743800E-01	0.2809700E-01	0.3760001E-03	0.3180001E-03
1.5250	0.3302600E-01	0.2814600E-01	0.2540001E-03	0.3920000E-03
1.5500	0.3783900E-01	0.2829100E-01	0.1210000E-03	0.4540000E-03
1.5750	0.4155900E-01	0.2854700E-01	-0.2199999E-04	0.5079999E-03
1.6000	0.4369500E-01	0.2887500E-01	-0.1670000E-03	0.5490000E-03
1.6250	0.4458900E-01	0.2922700E-01	-0.3060000E-03	0.5679999E-03
1.6500	0.4344600E-01	0.2957500E-01	-0.4230000E-03	0.5510000E-03
1.6750	0.4039000E-01	0.2991500E-01	-0.5010001E-03	0.4860000E-03
1.7000	0.3551100E-01	0.3022700E-01	-0.5290001E-03	0.3690000E-03
1.7250	0.2905700E-01	0.3047700E-01	-0.5010001E-03	0.2100000E-03
1.7500	0.2137000E-01	0.3064500E-01	-0.4230000E-03	0.3100000E-04
1.7750	0.1284800E-01	0.3074400E-01	-0.3100000E-03	-0.1390000E-03
1.8000	0.3913999E-02	0.3082400E-01	-0.1830000E-03	-0.2710000E-03
1.8250	-0.5038001E-02	0.3098300E-01	-0.6200001E-04	-0.3440001E-03
1.8500	-0.1374000E-01	0.3137300E-01	0.3500000E-04	-0.3519999E-03
1.8750	-0.2208700E-01	0.3212500E-01	0.9800000E-04	-0.3030000E-03
1.9000	-0.3002500E-01	0.3318900E-01	0.1250000E-03	-0.2170000E-03
1.9250	-0.3734500E-01	0.3418700E-01	0.1200000E-03	-0.1150000E-03
1.9500	-0.4356300E-01	0.3446300E-01	0.9000000E-04	-0.1700000E-04
1.9750	-0.4804200E-01	0.3337100E-01	0.4400000E-04	0.5300000E-04
2.0000	-0.5029800E-01	0.3061200E-01	-0.1000000E-04	0.1210000E-03
2.0250	-0.5025200E-01	0.2636900E-01	-0.6599999E-04	0.1590000E-03
2.0500	-0.4825000E-01	0.2111100E-01	-0.1140000E-03	0.1760000E-03
2.0750	-0.4487500E-01	0.1535000E-01	-0.1510000E-03	0.1820000E-03
2.1000	-0.4070600E-01	0.9404999E-02	-0.1690000E-03	0.1690000E-03
2.1250	-0.3617000E-01	0.3442000E-02	-0.1670000E-03	0.1370000E-03
2.1500	-0.3152000E-01	-0.2417000E-02	-0.1460000E-03	0.8599999E-04
2.1750	-0.2686700E-01	-0.8014001E-02	-0.1110000E-03	0.2100000E-04
2.2000	-0.2224100E-01	-0.1316500E-01	-0.7200000E-04	-0.5300000E-04
2.2250	-0.1764300E-01	-0.1769500E-01	-0.3500000E-04	-0.1270000E-03
2.2500	-0.1308600E-01	-0.2146400E-01	-0.8000000E-05	-0.1890000E-03
2.2750	-0.8622002E-02	-0.2436000E-01	0.8000000E-05	-0.2360000E-03
2.3000	-0.4335001E-02	-0.2630300E-01	0.1500000E-04	-0.2659999E-03
2.3250	-0.3350000E-03	-0.2725700E-01	0.2000001E-04	-0.2810000E-03
2.3500	0.3242000E-02	-0.2724500E-01	0.2799999E-04	-0.2860001E-03
2.3750	0.6248999E-02	-0.2635500E-01	0.4200000E-04	-0.2850001E-03
2.4000	0.0000000E 00	0.0000000E 00	0.0000000E 00	0.0000000E 00

Body fixed

$E_y(\ell, \ell_4 M r)$

$a = .5$

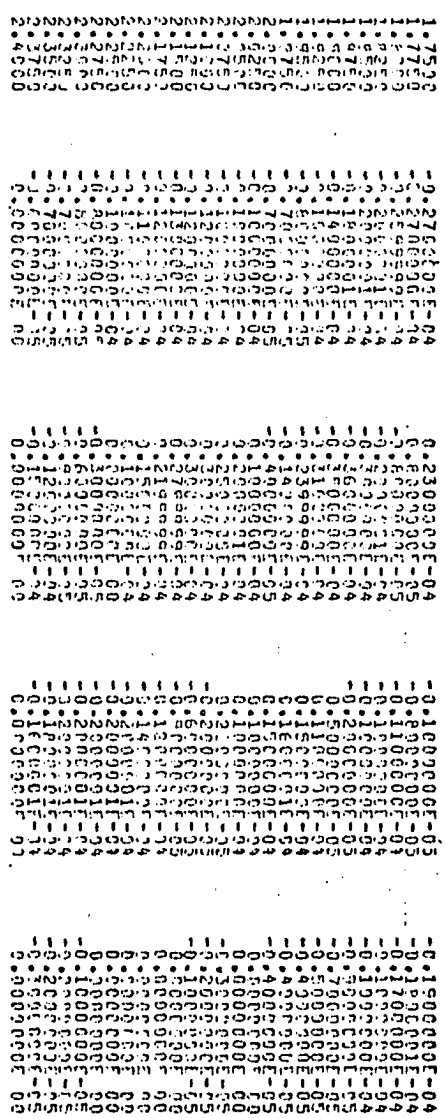
$T = 1.277$

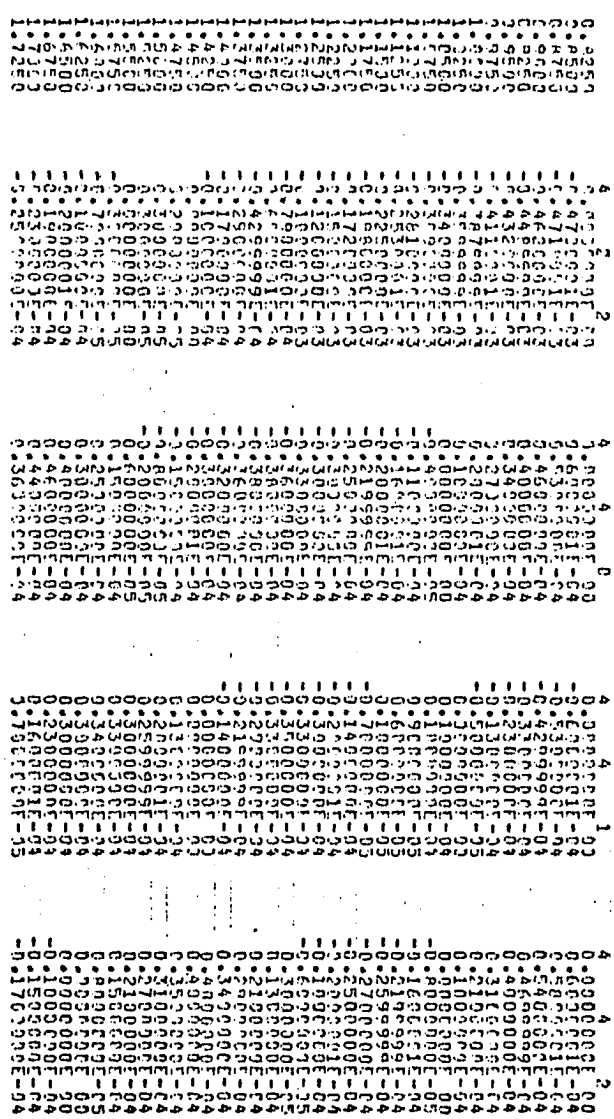
B·F

$E_y(l, l_2, r)$

$a = 0.5$

$T = 1.277$





Bf

Ej (l, l_2, n, r)

$Q = 0.5$

$T = 1.277$

BF
$\Omega = 0$
$E_j(\ell, l_z, r)$
$T = 1.294$

BF

$E_y(k, l, \omega = r)$

$Q = 1$

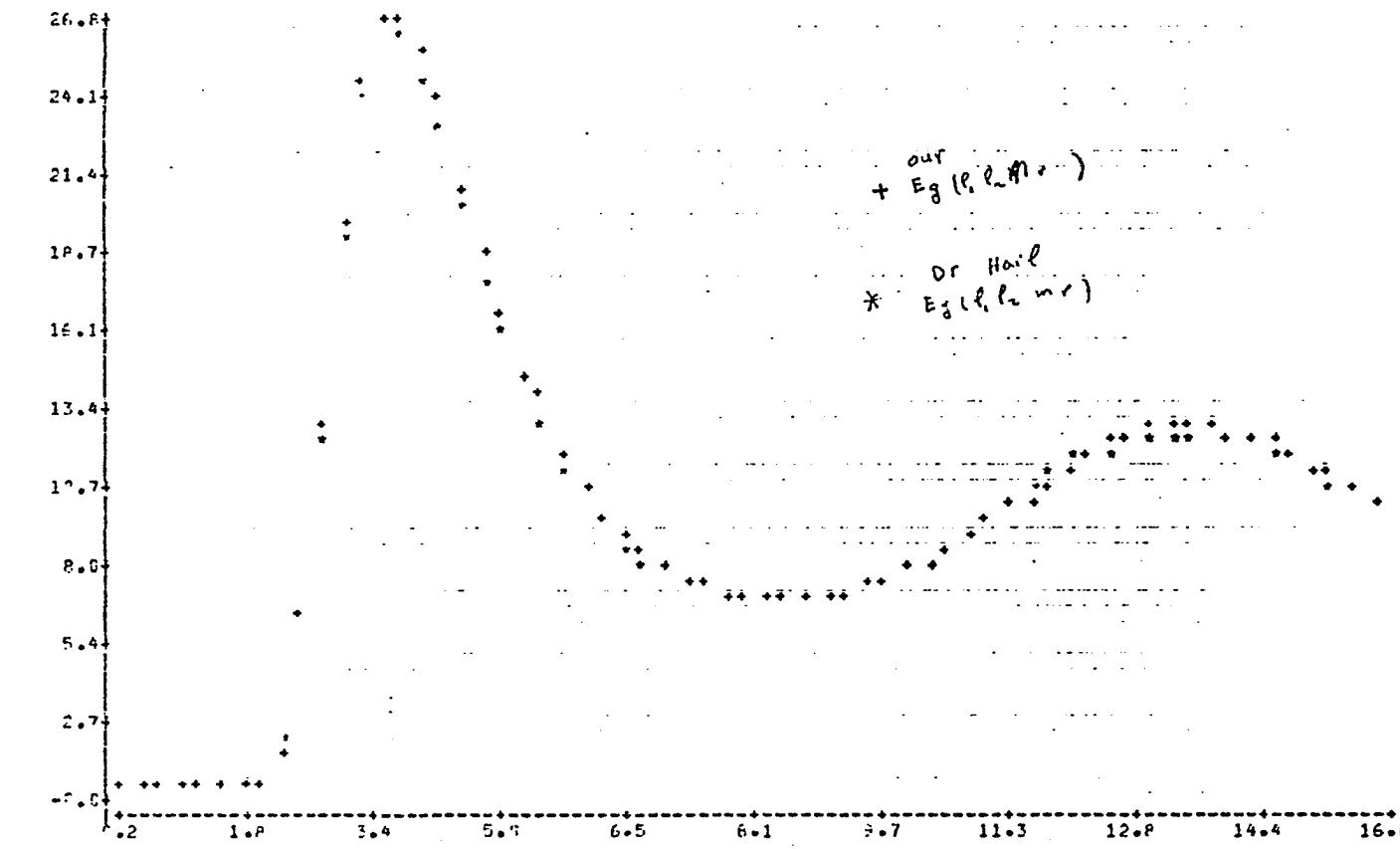
$T = 1.294$

B. F

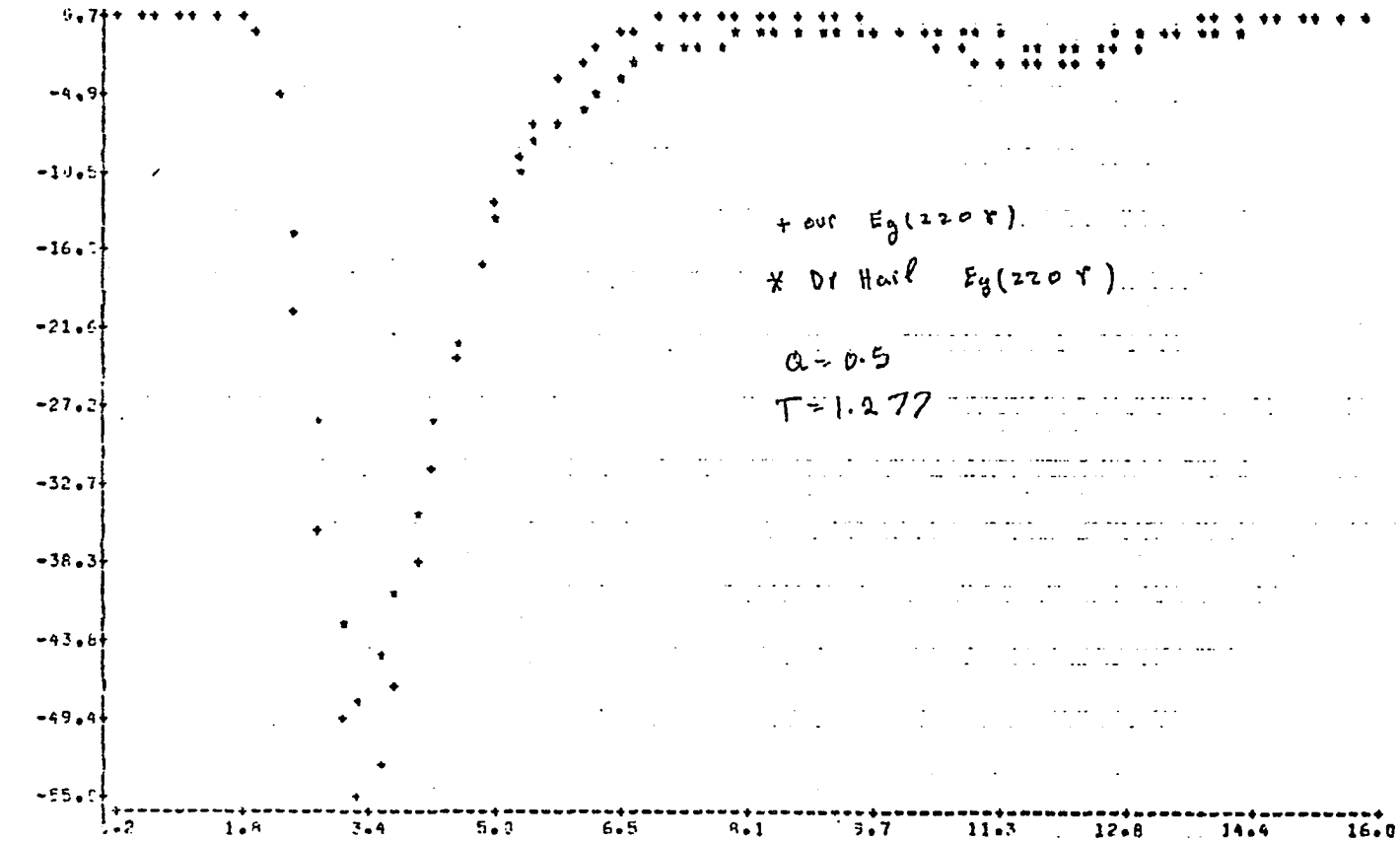
$E_y(l, l_2, m, r)$

$Q = 1$

$T = 1.294$



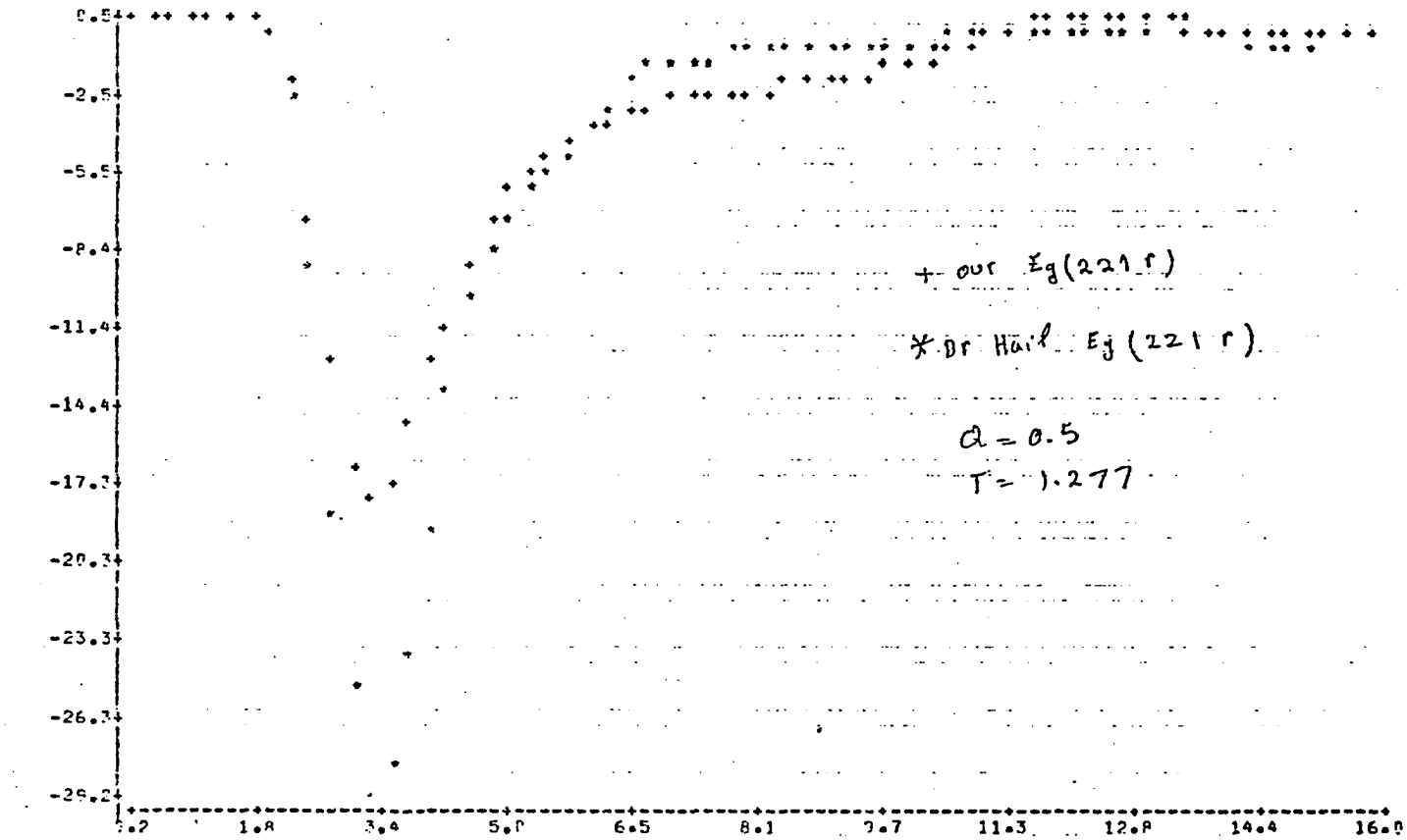
Eg(1000 r)
α = 0.5
T = 1.277



SCALE FACTOR USED IS 1.0E-02 * SCALE FACTOR USED IS 1.0E-01

IS EY$RUUUUUUUUUUUUUUUUU + IS UUUUUUUUUUUUUUUUUUUU

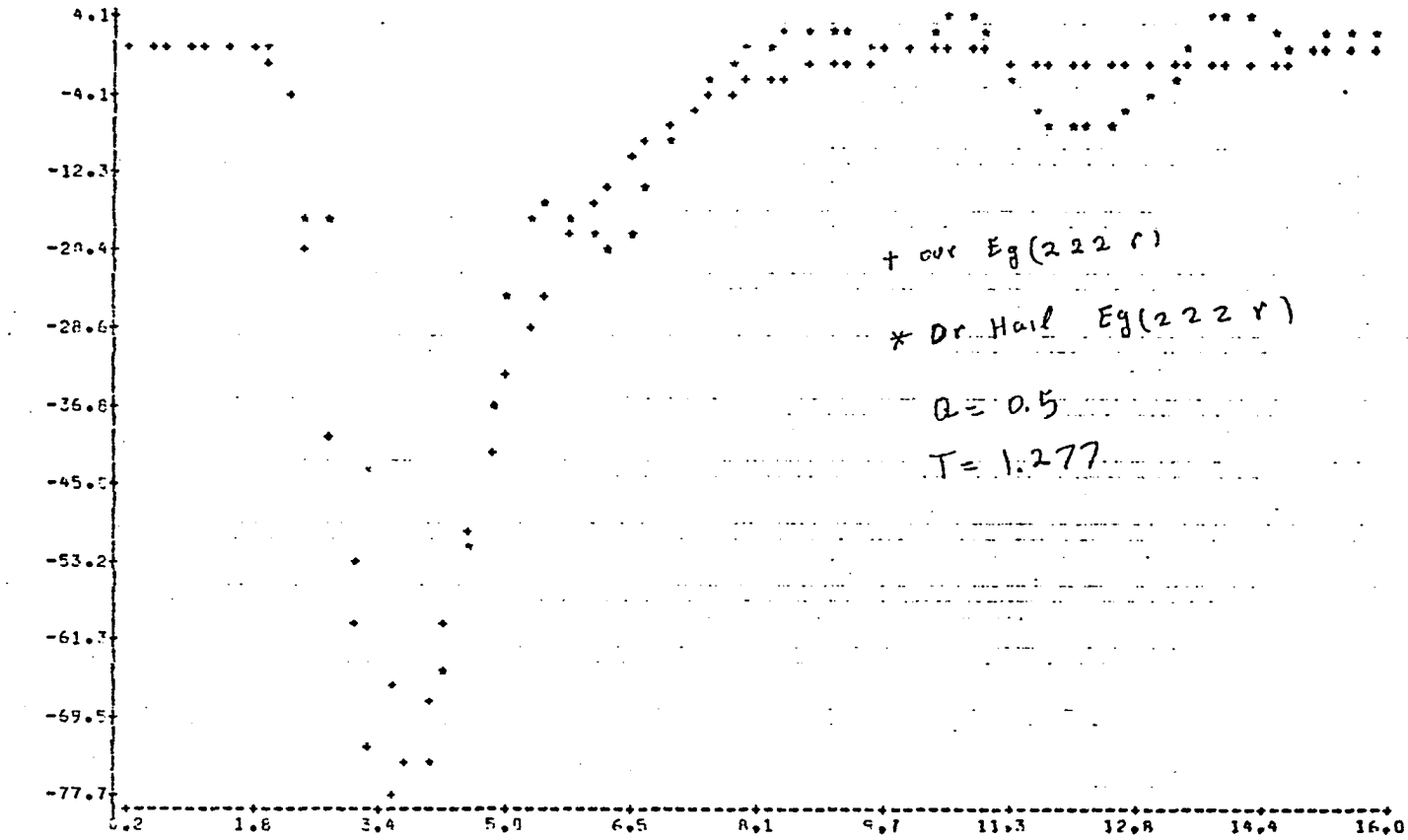
TATEMENTS EXECUTED= 32764



Y SCALE FACTOR USED IS 1.0E-02 X SCALE FACTOR USED IS 1.0E-01

* IS EY$RUUUUUUUUUUUUUUUU + IS UUUUUUUUUUUUUUUUUUU

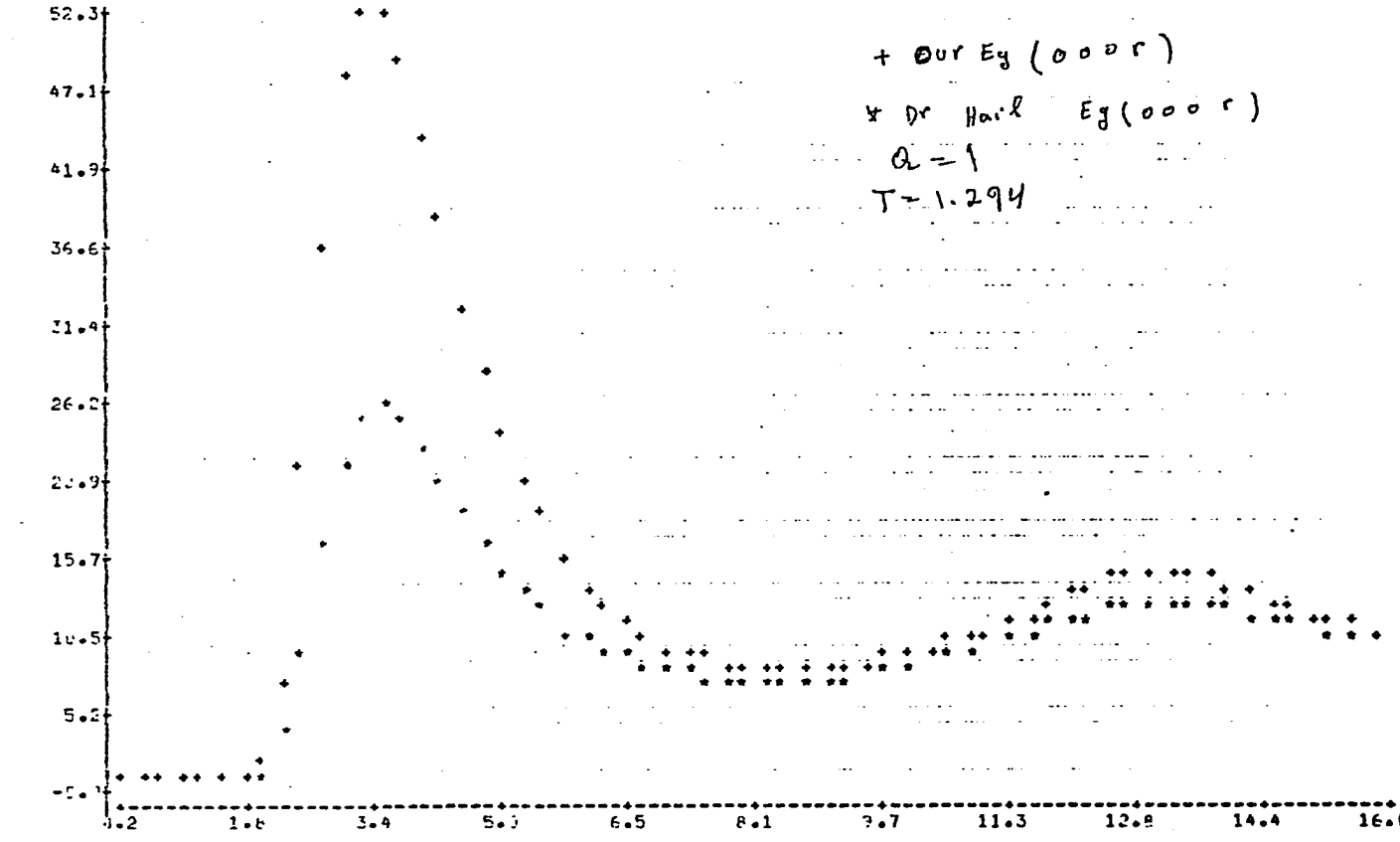
STATEMENTS EXECUTED= 32764

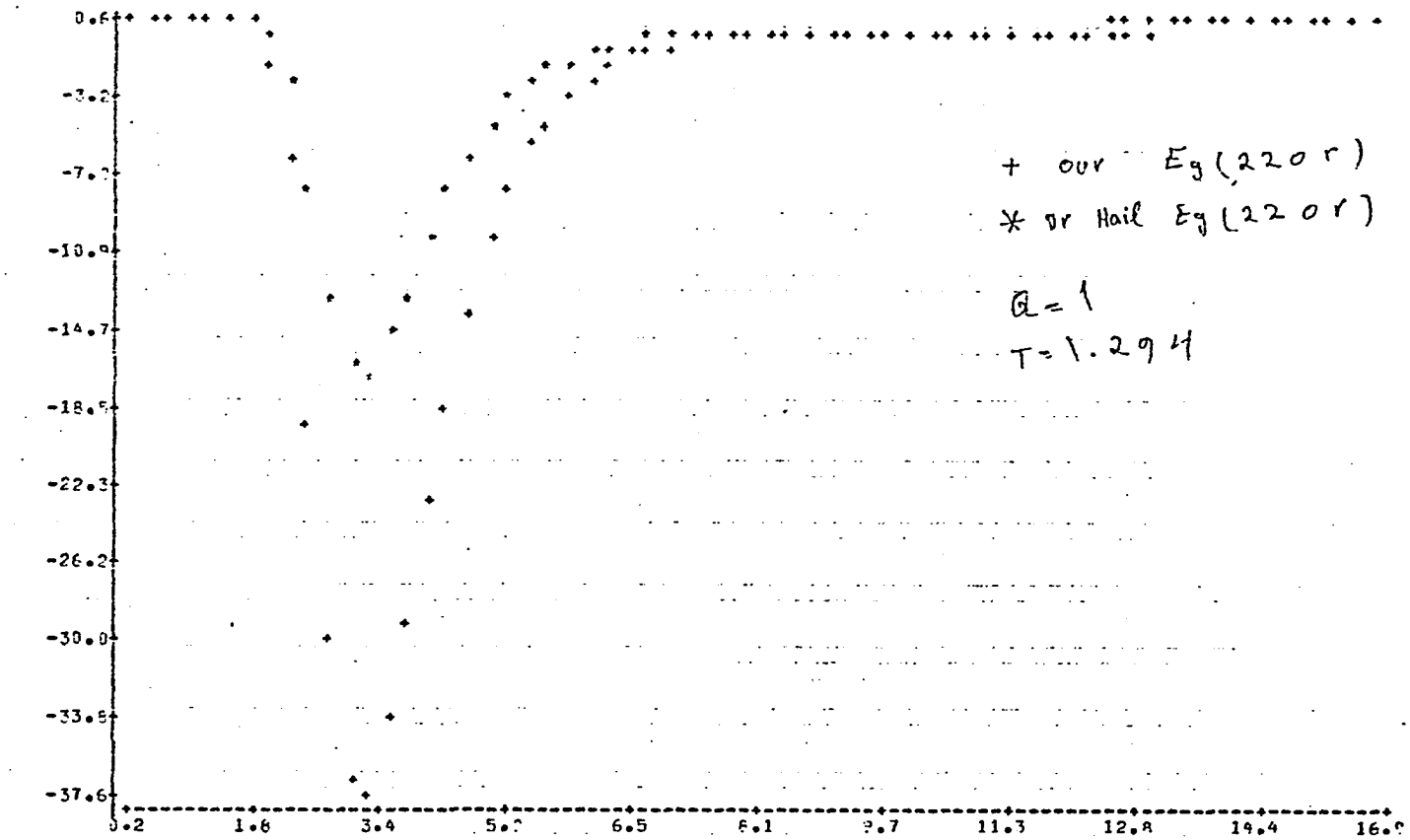


Y SCALE FACTOR USED IS 1.0E-03 X SCALE FACTOR USED IS 1.0E-01

* IS EYSRUUUUUUUUUUUUUUUUU + IS UUUUUUUUUUUUUUUUUUUU

STATEMENTS EXECUTED= 3276

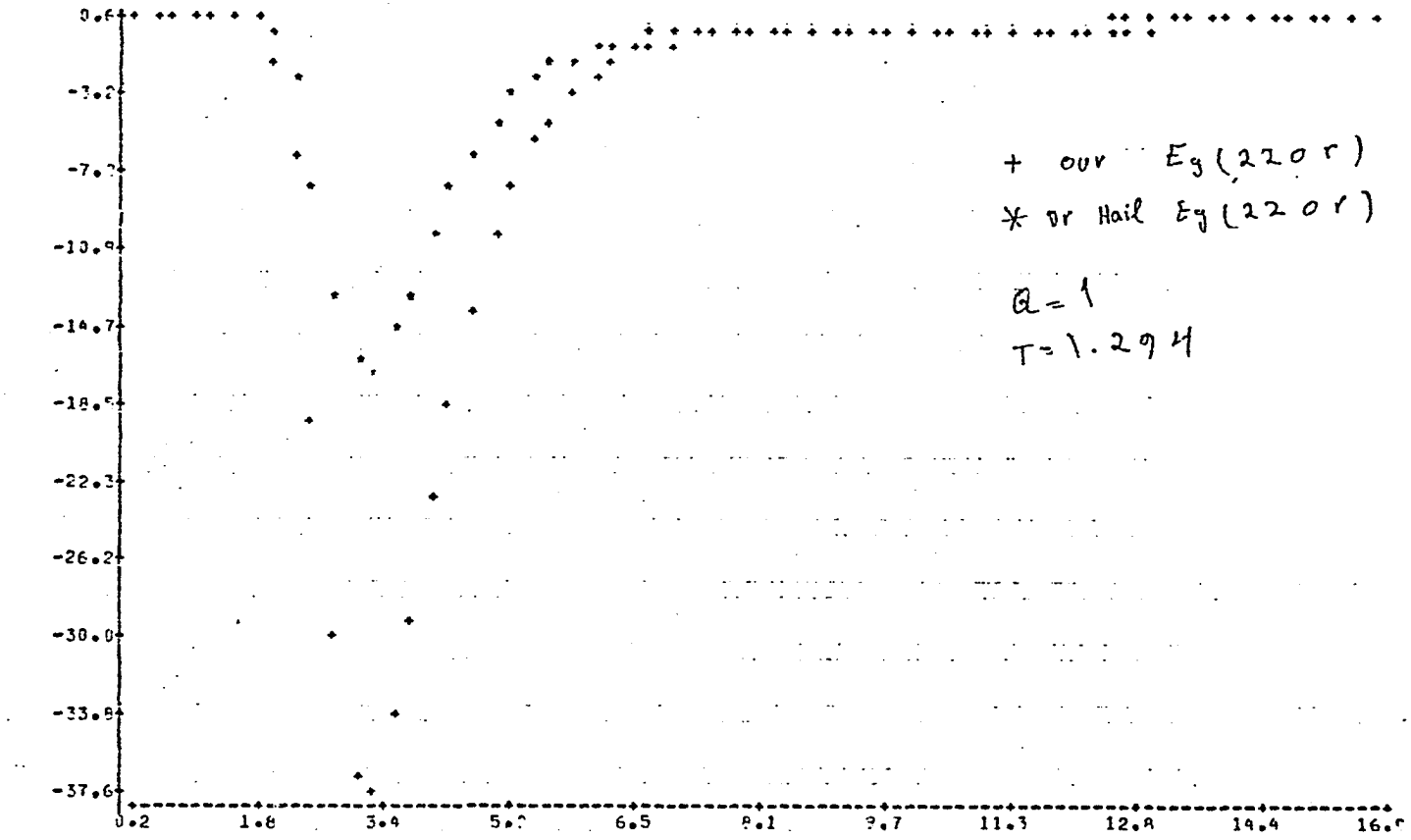

+ Our Eg (ooor)
* Dr Hail Eg(ooor)
Q=1
T=1.294
52.3
47.1
41.9
36.6
31.4
26.2
20.9
15.7
10.5
5.2
16.0
SCALE FACTOR USED IS 1.0E-01
X SCALE FACTOR USED IS 1.0E-01
TATEMENTS EXECUTED= 32760



Y SCALE FACTOR USED IS 1.0E-01 X SCALE FACTOR USED IS 1.0E-01

* IS EYEFUUUUUUUUUUUUUUUU + IS UUUUUUUUUUUUUUUUUUUU

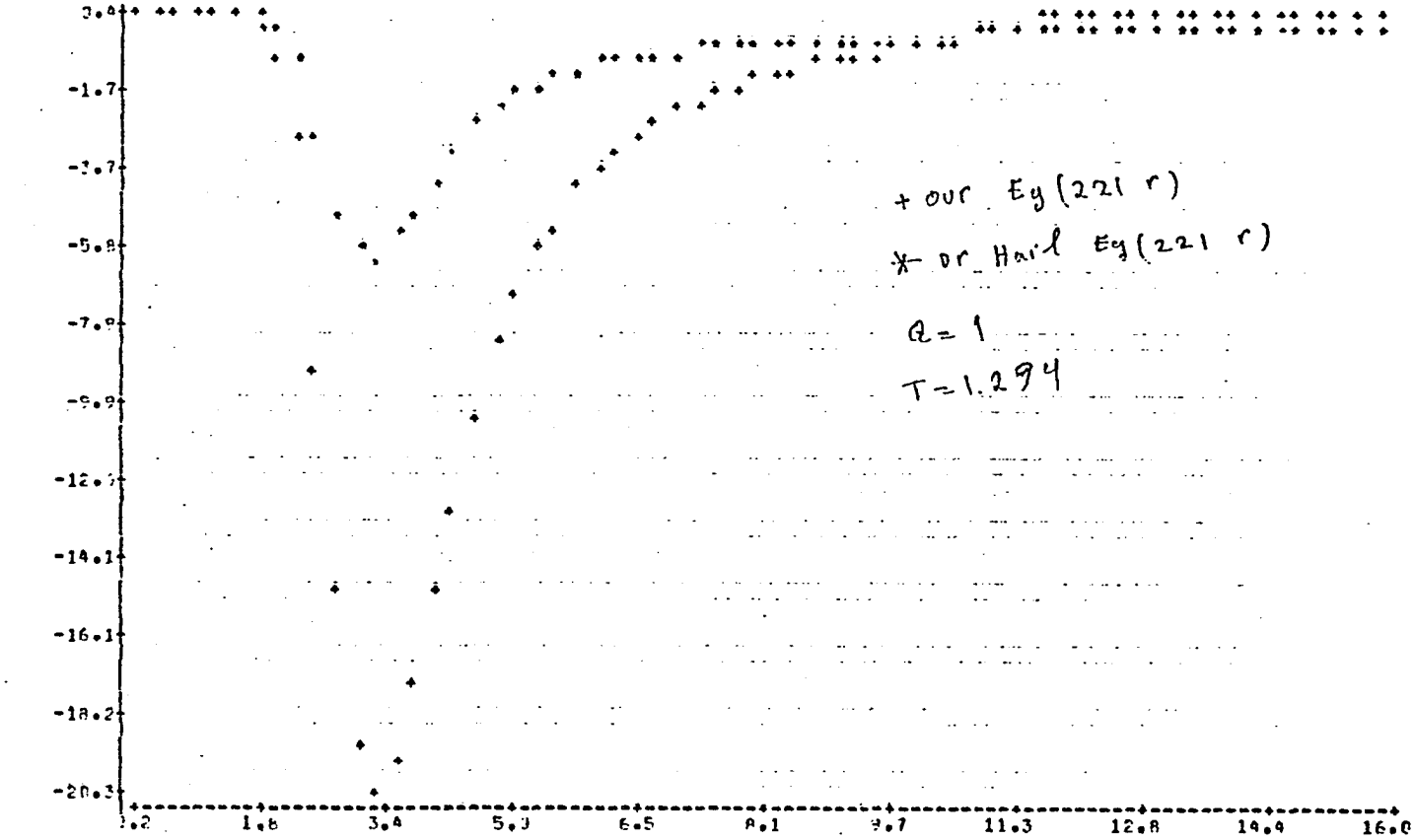
STATEMENTS EXECUTED= 32760



Y SCALE FACTOR USED IS 1.0E-01 X SCALE FACTOR USED IS 1.0E-01

* IS EYSFUUUUUUUUUUUUUUUU + IS UUUUUUUUUUUUUUUUUUUU

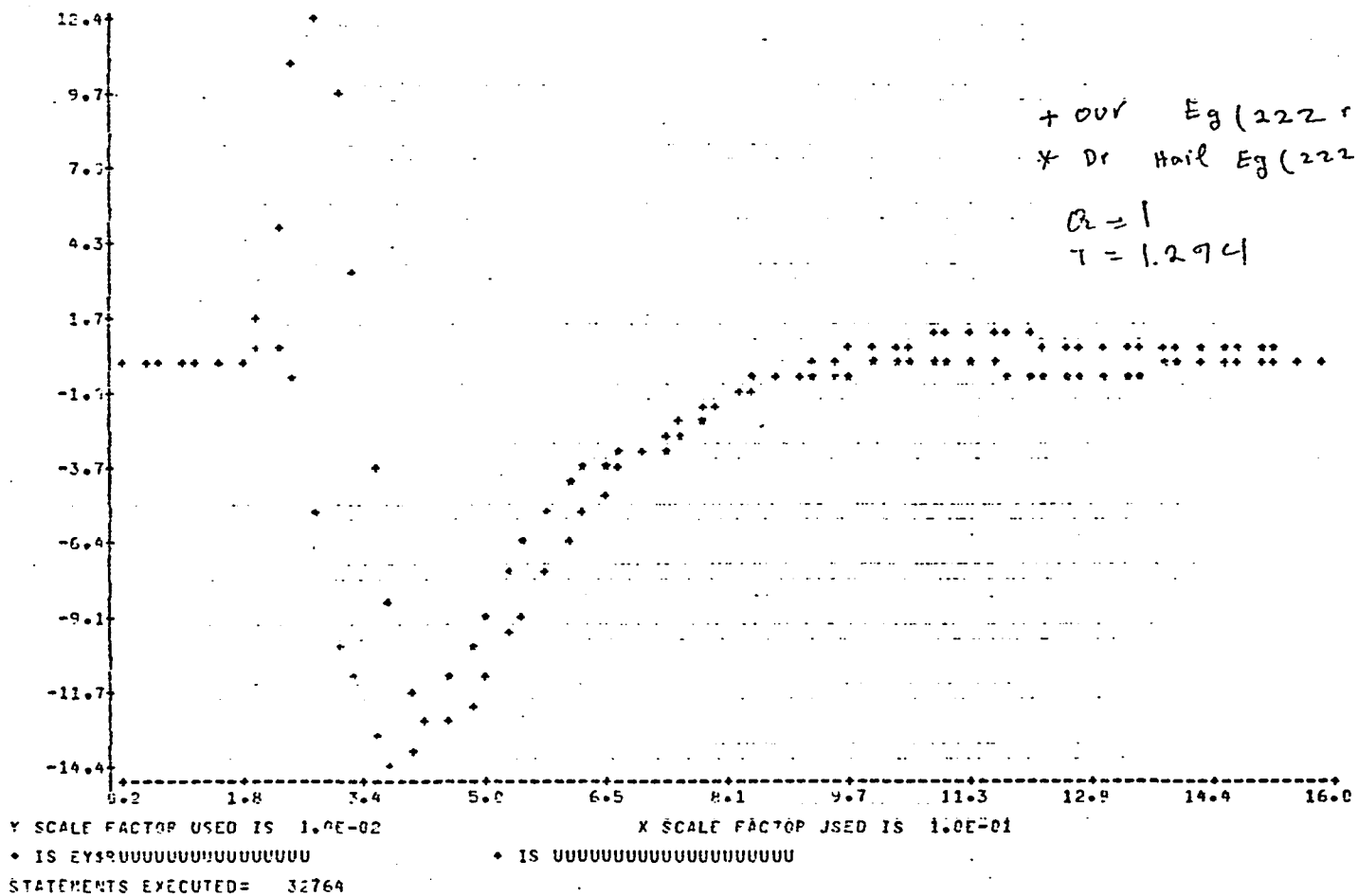
STATEMENTS EXECUTED= 32760



Y SCALE FACTOR USED IS 1.0E-01 X SCALE FACTOR USED IS 1.0E-01

+ IS EYSPUUUUUUUUUUUUUUUU + IS UUUUUUUUUUUUUUUUUUU

STATEMENTS EXECUTED= 32760


12.4
9.7
7.0
4.3
1.7
-1.0
-3.7
-6.4
-9.1
-11.7
-14.4
0.2
1.8
3.4
5.0
6.5
8.1
9.7
11.3
12.9
14.4
16.0
+ our Eg(222 r)
* Dr Hail Eg(222 r)
Q = 1
T = 1.294
Y SCALE FACTOR USED IS 1.0E-02
X SCALE FACTOR USED IS 1.0E+01
* IS EYSRUUUUUUUUUUUUUUUU
* IS UUUUUUUUUUUUUUUUUUUU
STATEMENTS EXECUTED= 32764

```
0001          CALL COMPA
0002          STOP
0003          END
```

```
FORTRAN IV G1  RELEASE 2.0            COMPA              DATE = 80213        02/14/12            PAGE 0001

0001                  SUBROUTINE COMPA
0002                  COMMON /CEYALL/ YNPUT(28,100)
0003                  COMMON /CG/ G(136)
0004                  COMMON /CEH/ EH(100)
0005                  COMMON/CLA/LA,LAP,MA,NB
0006                  COMMON /CPLOT/ X(100),Y(100,6)
0007                  DATA LAPL /*NAIL*/
0008                6 FORMAT(16I5)
0009               60 FORMAT(8F10.5)
0010               61 FORMAT (20F4.2)
0011               62 FORMAT (1X, 13G10.4)
0012               63 FORMAT (F10.5,F10.5, 6F10.6)
0013               64 FORMAT (10F8.3)
0014               65 FORMAT (1X, 130('*'))
0015               66 FORMAT ( 1H1)
0016                  NP=40
0017                  NB=60
0018                  NF=6
0019                  NY=100
0020                  NG=40
0021                  NP=64
0022                  NC=64
0023                  NY=64
0024                  NF=64
0025                  READ (5,6 ) NFOIS
0026                  WRITE(6,6 ) NFOIS
0027                  READ (5,60) (G(I), I=1,NG)
0028                  WRITE(6,64) (G(I), I=1,NG)
0029                  DO 4 INPUT=1,14
0030                  READ (5,6)      K1,K2,K3
0031                  WRITE(6,6)      K1,K2,K3
0032                  READ (5,60) (YNPUT (INPUT,I), I=1,NF)
0033                  WRITE(6,61) (YNPUT (INPUT,I), I=1,NF)
0034                4 CONTINUE
0035                  DO 41 K=1,NF
0036                  YNPUT(1,K)=YNPUT(1,K) +1.
0037               41 CONTINUE
0038                  DO 456 INPUT=15,28
0039                  READ (5,6)      K1,K2,K3
0040                  WRITE (6,6) K1,K2,K3
0041                  READ (5,60) (YNPUT (INPUT,I), I=2,NY)
0042                  WRITE(6,61) (YNPUT (INPUT,I), I=2,NY)
0043              456 CONTINUE
0044                  DO 4981 II=1,NFOIS
0045                  READ (5,6 ) LA, LAP, MA
0046                  WRITE (6,66)
0047                  WRITE(6,6 ) LA, LAP, MA
0048                  WRITE (6,65)
0049                  DO 40 NPOINT=1,NB
0050                  CALL HAILE (NPOINT)
0051               40 CONTINUE
0052                  WRITE (6,65)
0053                  WRITE (6,66)
0054                  WRITE (7,6) LA, LAP, MA
0055                  WRITE (6,65)
0056                  WRITE (6,62) (EH(I), I=1,NP)
0057                  WRITE (6,65)
0058                  WRITE (7,63) (EH(I), I=1,NP)
```

92

```
0059                  DO 472 II=1,100
0060                  X(II) =(II-19.)*0.025
0061            472   Y(II,1)= EH(II)
0062                  CALL PRPLOT (X, Y, 100, 6, 90, 6   , LABL)
0063          4001    CONTINUE
0064                  RETURN
0065                  END
```

```
FORTRAN IV G1  RELEASE 2.0          HAILE          DATE = 80213      03/14/12          PAGE 0001

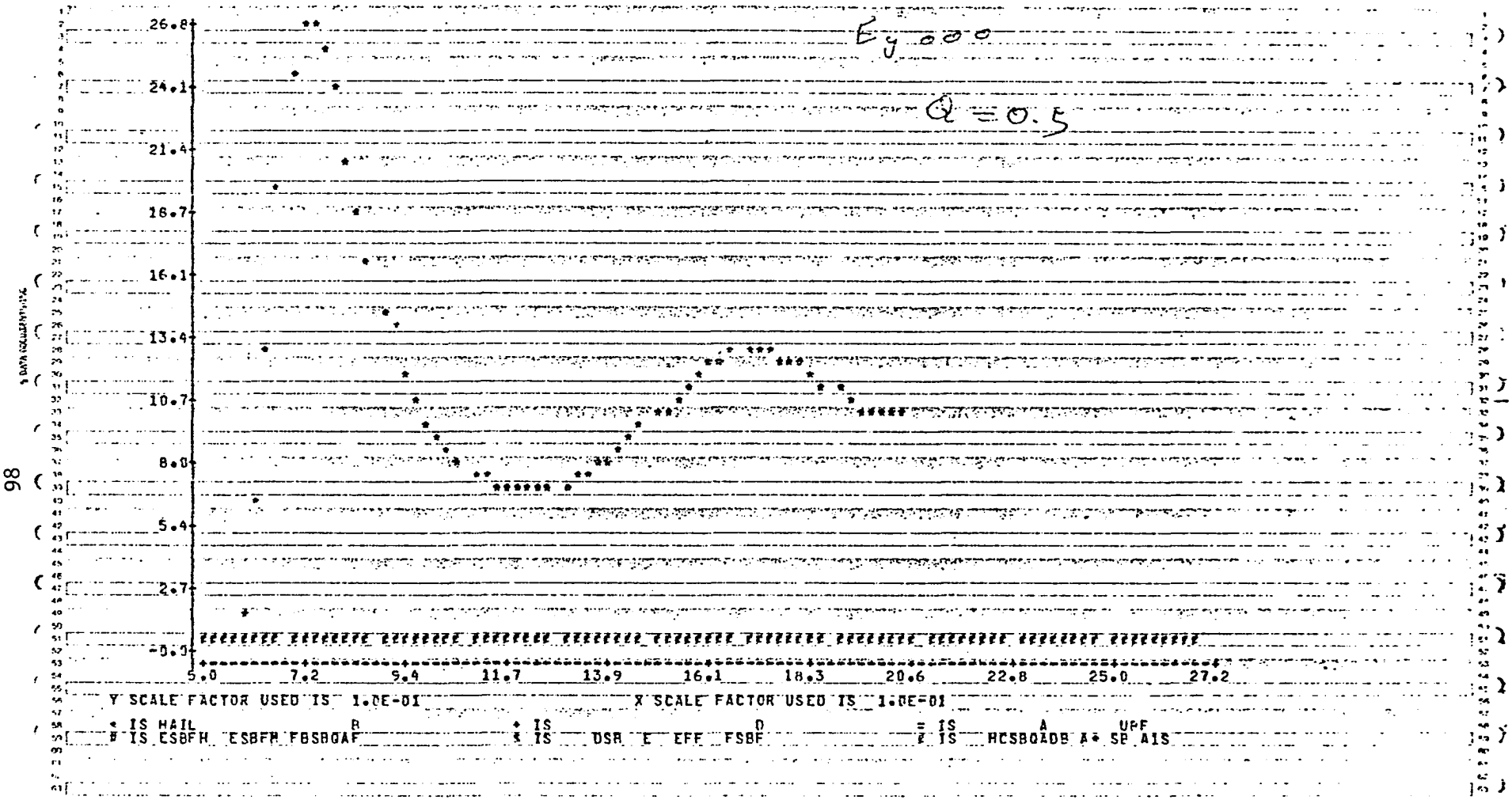
0001                  SUBROUTINE HAILE    (NPOINT)
0002                  COMMON /CEYALL/ YNPUT(28,100)
0003                  COMMON /CEH/ EH(103)
0004                  COMMON /CG/ G(106)
0005                  DIMENSION EU(7,7,7), EY(7,7,7)
0006                  COMMON /CLA/LA, LAP, MA ,NB
0007                6 FORMAT (8F10.5)
0008               60 FORMAT (1615)
0009               61 FORMAT (3X, I5, F8.3,2X,G15.7,9X,3G12.5)
0010                  MAP=-MA
0011                  EU(1,1,1) =YNPUT(1,NPOINT)
0012                  EY(1,1,1) =YNPUT(15,NPOINT)
0013                  EU(3,1,1) =YNPUT(2,NPOINT)
0014                  EY(3,1,1) =YNPUT(16,NPOINT)
0015                  EU(5,1,1) =YNPUT(3,NPOINT)
0016                  EY(5,1,1) =YNPUT(17,NPOINT)
0017                  EU(3,3,1) =YNPUT(4,NPOINT)
0018                  EY(3,3,1) =YNPUT(18,NPOINT)
0019                  EU(3,3,2) =YNPUT(5,NPOINT)
0020                  EY(3,3,2) =YNPUT(19,NPOINT)
0021                  EU(3,3,3) =YNPUT(6,NPOINT)
0022                  EY(3,3,3) =YNPUT(20,NPOINT)
0023                  EU(5,3,1) =YNPUT(7,NPOINT)
0024                  EY(5,3,1) =YNPUT(21,NPOINT)
0025                  EU(5,3,2) =YNPUT(8,NPOINT)
0026                  EY(5,3,2) =YNPUT(22,NPOINT)
0027                  EU(5,3,3) =YNPUT(9,NPOINT)
0028                  EY(5,3,3) =YNPUT(23,NPOINT)
0029                  EU(5,5,1) =YNPUT(10,NPOINT)
0030                  EY(5,5,1) =YNPUT(24,NPOINT)
0031                  EU(5,5,2) =YNPUT(11,NPOINT)
0032                  EY(5,5,2) =YNPUT(25,NPOINT)
0033                  EU(5,5,3) =YNPUT(12,NPOINT)
0034                  EY(5,5,3) =YNPUT(26,NPOINT)
0035                  EU(5,5,4) =YNPUT(13,NPOINT)
0036                  EY(5,5,4) =YNPUT(27,NPOINT)
0037                  EU(5,5,5) =YNPUT(14,NPOINT)
0038                  EY(5,5,5) =YNPUT(28,NPOINT)
0039                  SUM=0.
0040                  DO 4 NLP=1,5,2
0041                  LP=NLP-1
0042                  DO 4 NLXP=1,5,2
0043                   LXP=NLXP-1
0044                  SIZE=1.
0045                  DO 41NL=NLP,5,2
0046                  L=NL-1
0047                  TAILLE=1.
0048                  DO 42 NLX=NLXP,5,2
0049                  LX=NLX-1
0050                  LAGEUR=(2*L +1)*(2*LX+1)*(2*LP+1)*(2*LXP+1)
0051                  A=LAGEUR
0052                  A=A/(2.*LA+1)/(2.*LAP+1)
0053                  Q=SQRT(A)
0054                  MMAX=MIN0(NL,NLP)
0055                  MXMAX=MIN0(NLX,NLXP)
0056                  MAXM=2 *MMAX-1
0057                  MAXMX= 2*MXMAX-1
0058                  DO 40 MM=1, MAXM
```

```
      M =NM=MMAX
      MP=-M
      DO 40 NMX=1, MAXMX
      MX = NMX -MXMAX
      MXP=-MX
      LM=IABS(M)+1
      LMX=IABS(MX)+1
      SUM=SUM+EU(NL,NLP,LM)*EY(NLX,NLXP,LMX)*C(L,LX,LA,M,MX,MA)
     1 *C(L,LY,LA,0,0,0)*C(LP,LXP,LAP,MP,MXP,MAP)*C(LP,LXP,LAP,0,0,0)*0
     2 *SIZE *TAILLE
   40 CONTINUE
      TAILLE=2.
   42 CONTINUE
      SIZE=2.
   41 CONTINUE
    4 CONTINUE
      NLA=LA+1
      NLAP=LAP+1
      NMA=MA+1
      EH(NPOINT)= G(NPOINT)*SUM + G(NPOINT)*EU(NLA,NLAP,NMA)
      R12= NPOINT*0.025 +0.775
      WRITE (6,61) NPOINT, R12, EH(NPOINT), SUM,G(NPOINT),EU(NLA,NLAP,
     1 NMA)
      RETURN
      END
```

```
0001            FUNCTION C(J1,J2,J3,M1,M2,MM33)
0002            C=0.
0003            M3=M1+M2
0004            IF (M3 .NE. MM33) RETURN
0005            K1=2*J3+1
0006            K2=J3+J1-J2
0007            K3=J3-J1+J2
0008            K4=J1+J2-J3
0009            K5=J3+M3
0010            K6=J3-M3
0011            K7=J1+J2+J3+1
0012            K8=J1-M1
0013            K9=J1+M1
0014            K10=J2-M2
0015            K11=J2+M2
0016            IF (K1.LT.0 .OR. K2.LT.0 .OR. K3.LT.0 .OR. K4.LT.0 .OR. K5.LT.0
               1 .OR. K6.LT.0 .OR. K7.LT.0 .OR. K8.LT.0 .OR. K9.LT.0 .OR. K10.LT.0
               2 .OR. K11.LT.0) RETURN
0017            R1=FACT(K2)*FACT(K3)*FACT(K4)*FACT(K5)*FACT(K6)
0018            R2=FACT(K8)*FACT(K9)*FACT(K10)*FACT(K11)
0019            R3=FACT(K7)
0020            DOWN=(K1*R1*R2+0.0)/R3
0021            FIRST=SQRT(DOWN)
0022            MAX=IABS(J1)+IABS(J2) +IABS(J3)+1
0023            SUM=0.
0024            DO 40 NEU=1, MAX
0025            NEU=NEU-1
0026            L1=J1+J2-J3-NEU
0027            L2=J1-M1-NEU
0028            L3=J2+M2-NEU
0029            L4=J3-J2+M1+NEU
0030            L5=J3-J1-M2+NEU
0031            IF (L1.LT.0 .OR. L2.LT.0 .OR. L3.LT.0 .OR. L4.LT.0 .OR. L5.LT.0)
               1GO TO 40
0032            UP=(-1)**NEU*FACT(L1)*FACT(L2)*FACT(L3)*FACT(L4)*FACT(L5)*FACT(NEU
               1 )
0033            SUM=SUM +1./UP
0034       40   CONTINUE
0035            C =FIRST*SUM
0036            RETURN
0037            END
```

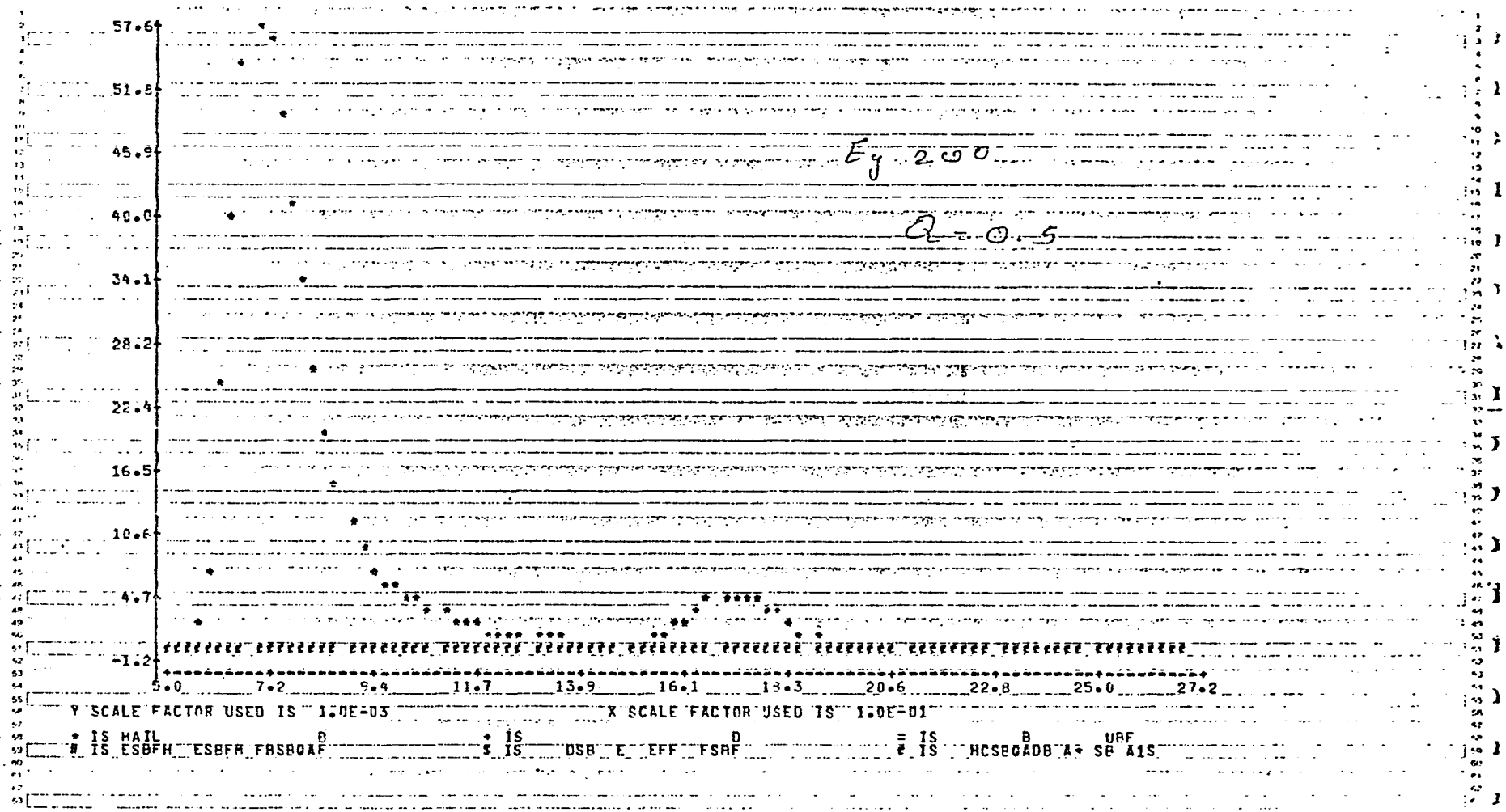
```
FORTRAN IV G1  RELEASE 2.0          FACT          DATE = 80213      03/14/12          PAGE 0001

0001                    FUNCTION FACT(N)
0002                    FACT=1.
0003                    IF (N .LE. 0) GO TO 7
0004                    U=1.
0005                    DO 4 I=1,N
0006                  4 U=U*I
0007                    FACT=U
0008                  7 RETURN
0009                    END
```


Eyooo
Q=0.5
26.8
24.1
21.4
16.7
16.1
13.4
10.7
8.0
5.4
2.7
-0.0
5.0
7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Y SCALE FACTOR USED IS 1.0E-01
X SCALE FACTOR USED IS 1.0E-01
* IS HAIL B * IS D = IS A UPF
# IS ESBFH ESBFM FBSBQAF % IS DSR E EFF FSBF # IS HCSBQADB A* SP A1S

Eg 2 — Q=0.5

1	0.800	.0	.0	.0	.0	.18827
2	0.825	.0	.0	.0	.0	.15137
3	0.850	.0	.0	.42807E-03	.0	.11948
4	0.875	.0	.0	.78859E-03	.0	.76559E-01
5	0.900	.17088613E-02	.20861E-02	.28250E-01	.58415E-01	
6	0.925	.69011822E-02	.36799E-02	.13500	.47440E-01	
7	0.950	.2357920E-01	.49E16E-02	.59123	.34920E-01	
8	0.975	.3992320E-01	.62415E-02	1.1880	.27260E-01	
9	1.000	.5309767E-01	.72549E-02	1.8462	.21460E-01	
10	1.025	.5763656E-01	.79209E-02	2.3174	.16954E-01	
11	1.050	.5584795E-01	.82305E-02	2.5736	.13470E-01	
12	1.075	.4927321E-01	.81819E-02	2.6013	.10760E-01	
13	1.100	.4001120E-01	.78603E-02	2.4757	.86200E-02	
14	1.125	.3363700E-01	.73170E-02	2.3090	.72500E-02	
15	1.150	.2500369E-01	.66754E-02	2.0377	.56200E-02	
16	1.175	.1904203E-01	.59673E-02	1.8008	.45600E-02	
17	1.200	.1437419E-01	.52837E-02	1.5970	.37200E-02	
18	1.225	.1095380E-01	.46835E-02	1.4182	.30400E-02	
19	1.250	.9111899E-02	.41673E-02	1.3230	.27000E-02	
20	1.275	.6808426E-02	.39603E-02	1.1309	.20600E-02	
21	1.300	.5619698E-02	.38078E-02	1.0202	.17000E-02	
22	1.325	.4899967E-02	.37042E-02	.94700	.14700E-02	
23	1.350	.4144908E-02	.36312E-02	.86332	.11700E-02	
24	1.375	.3587281E-02	.34683E-02	.80644	.98000E-03	
25	1.400	.3053762E-02	.32087E-02	.75800	.82000E-03	
26	1.425	.2556420E-02	.28711E-02	.71787	.69000E-03	
27	1.450	.2146585E-02	.24509E-02	.69900	.62000E-03	
28	1.475	.1721473E-02	.20635E-02	.67417	.49000E-03	
29	1.500	.1382741E-02	.16681E-02	.66538	.41000E-03	
30	1.525	.1098750E-02	.12992E-02	.66100	.36000E-03	
31	1.550	.8433922E-03	.99138E-03	.65226	.30000E-03	
32	1.575	.6402705E-03	.71699E-03	.65535	.26000E-03	
33	1.600	.4666371E-03	.47961E-03	.66700	.22000E-03	
34	1.625	.3114720E-03	.26568E-03	.68354	.19000E-03	
35	1.650	.1768513E-03	.84097E-04	.69600	.17000E-03	
36	1.675	.5093509E-04	-.70415E-04	.73199	.14000E-03	
37	1.700	-.6326417E-04	-.20272E-03	.76466	.12000E-03	
38	1.725	-.1618703E-03	-.31387E-03	.79400	.11000E-03	
39	1.750	-.2671711E-03	-.40863E-03	.83950	.99000E-04	
40	1.775	-.3536650E-03	-.48211E-03	.87803	.83000E-04	
41	1.800	-.4035521E-03	-.50909E-03	.92300	.70000E-04	
42	1.825	-.3878656E-03	-.46206E-03	.96478	.60000E-04	
43	1.850	-.2273453E-03	-.27916E-03	.99200	.50000E-04	
44	1.875	.7571797E-04	.31877E-04	1.0534	.40000E-04	
45	1.900	.6023697E-03	.51009E-03	1.0950	.40000E-04	
46	1.925	.1330897E-02	.11170E-02	1.1270	.40000E-04	
47	1.950	.2137462E-02	.17899E-02	1.1745	.30000E-04	
48	1.975	.2971854E-02	.24406E-02	1.2029	.30000E-04	
49	2.000	.3649164E-02	.29711E-02	1.2200	.20000E-04	
50	2.025	.4080683E-02	.32982E-02	1.2298	.20000E-04	
51	2.050	.4219139E-02	.34046E-02	1.2320	.20000E-04	
52	2.075	.4047755E-02	.32795E-02	1.2268	.20000E-04	
53	2.100	.3641096E-02	.29729E-02	1.2163	.20000E-04	
54	2.125	.3069352E-02	.25412E-02	1.2030	.10000E-04	
55	2.150	.2400902E-02	.20380E-02	1.1719	.10000E-04	
56	2.175	.1727389E-02	.15016E-02	1.1428	.10000E-04	
57	2.200	.1092173E-02	.96319E-03	1.1120	.10000E-04	
58	2.225	.4938005E-03	.44849E-03	1.0770	.10000E-04	
59	2.250	-.1995919E-04	-.26901E-04	1.0560	.10000E-04	
60	2.275	-.4975614E-03	-.41245E-03	1.0127	.10000E-04	
61	2.300	-.6987636E-03	-.71867E-03	.98602	.10000E-04	
62	2.325	-.8985465E-03	-.93921E-03	.96700	.10000E-04	
63	2.350	-.1048281E-02	-.10941E-02	.96700	.10000E-04	
64	2.375	-.1163305E-02	-.12130E-02	.96700	.10000E-04	


57.6
51.8
46.0
40.0
34.1
28.2
22.4
16.5
10.6
4.7
-1.2
5.0
7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Eg 200
Q=0.5
Y SCALE FACTOR USED IS 1.0E-03
X SCALE FACTOR USED IS 1.0E-01
* IS HAIL
# IS ESBFH ESBFM FRSBOAF
+ IS
$ IS DSB E EFF FSBF
= IS
@ IS HCSBOADB A+ SB A1S

Eg 4 c c

Q = 0.5

1	0.600	.0	.0	.0	.10644
2	0.625	.0	.0	.0	.82830E-01
3	0.650	.0	.71139E-01	.0	.59220E-01
4	0.675	.0	.53799E-01	.0	.37396E-01
5	0.900	.20154758E-02	.43754E-01	.28250E-01	.27590E-01
6	0.925	.78960556E-02	.36519E-01	.13500	.21970E-01
7	0.950	.26140115E-01	.28473E-01	.59123	.15740E-01
8	0.975	.41225935E-01	.22612E-01	1.1880	.12090E-01
9	1.000	.49911665E-01	.17657E-01	1.8460	.93800E-02
10	1.025	.48093321E-01	.13433E-01	2.3174	.73200E-02
11	1.050	.40172216E-01	.98495E-02	2.5736	.57600E-02
12	1.075	.29457698E-01	.67644E-02	2.6013	.45600E-02
13	1.100	.19235259E-01	.41396E-02	2.4757	.36300E-02
14	1.125	.11669941E-01	.20225E-02	2.3090	.30400E-02
15	1.150	.68668861E-02	.48447E-04	2.0377	.23400E-02
16	1.175	.70128571E-03	-.15023E-02	1.8088	.18900E-02
17	1.200	-.19661259E-02	-.27691E-02	1.5970	.15400E-02
18	1.225	-.35846640E-02	-.37777E-02	1.4182	.12500E-02
19	1.250	-.46016311E-02	-.45082E-02	1.3230	.11100E-02
20	1.275	-.48629947E-02	-.51577E-02	1.1709	.84000E-03
21	1.300	-.49618077E-02	-.55636E-02	1.0202	.70000E-03
22	1.325	-.49564439E-02	-.58338E-02	.94700	.60000E-03
23	1.350	-.46696748E-02	-.58690E-02	.86332	.48000E-03
24	1.375	-.43685515E-02	-.58418E-02	.80644	.40000E-03
25	1.400	-.40566897E-02	-.56021E-02	.75609	.33600E-03
26	1.425	-.36927477E-02	-.54240E-02	.71787	.28000E-03
27	1.450	-.34467704E-02	-.51723E-02	.69900	.25000E-03
28	1.475	-.30693903E-02	-.47527E-02	.67417	.20000E-03
29	1.500	-.27899695E-02	-.43630E-02	.66538	.17300E-03
30	1.525	-.25301085E-02	-.39777E-02	.66100	.15000E-03
31	1.550	-.22331935E-02	-.35406E-02	.65286	.12000E-03
32	1.575	-.19891147E-02	-.31215E-02	.65535	.10000E-03
33	1.600	-.17439925E-02	-.27047E-02	.66700	.90000E-04
34	1.625	-.15089965E-02	-.22876E-02	.68354	.80700E-04
35	1.650	-.12725808E-02	-.18984E-02	.69600	.70000E-04
36	1.675	-.10595511E-02	-.14974E-02	.73199	.60000E-04
37	1.700	-.82927159E-03	-.11242E-02	.76486	.48000E-04
38	1.725	-.58493188E-03	-.77669E-03	.79400	.40000E-04
39	1.750	-.35972306E-03	-.44827E-03	.83850	.30000E-04
40	1.775	-.10113588E-03	-.14516E-03	.87803	.30000E-04
41	1.800	.16397577E-03	.14023E-03	.92000	.30000E-04
42	1.825	.44406077E-03	.44027E-03	.96478	.20000E-04
43	1.850	.76976288E-03	.75597E-03	.99200	.20000E-04
44	1.875	.11030198E-02	.11030E-02	1.0534	.20000E-04
45	1.900	.16514088E-02	.14082E-02	1.0950	.20000E-04
46	1.925	.21611536E-02	.19076E-02	1.1270	.10000E-04
47	1.950	.27431046E-02	.23256E-02	1.1795	.10000E-04
48	1.975	.32840508E-02	.27201E-02	1.2029	.10000E-04
49	2.000	.37325689E-02	.30495E-02	1.2200	.10000E-04
50	2.025	.40390866E-02	.32744E-02	1.2298	.10000E-04
51	2.050	.41966285E-02	.33966E-02	1.2320	.10000E-04
52	2.075	.41615955E-02	.33823E-02	1.2268	.10000E-04
53	2.100	.39713055E-02	.32552E-02	1.2163	.10000E-04
54	2.125	.36567953E-02	.30297E-02	1.2030	.10000E-04
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62	2.325	.20692288E-03	.21398E-03	.96700	.0
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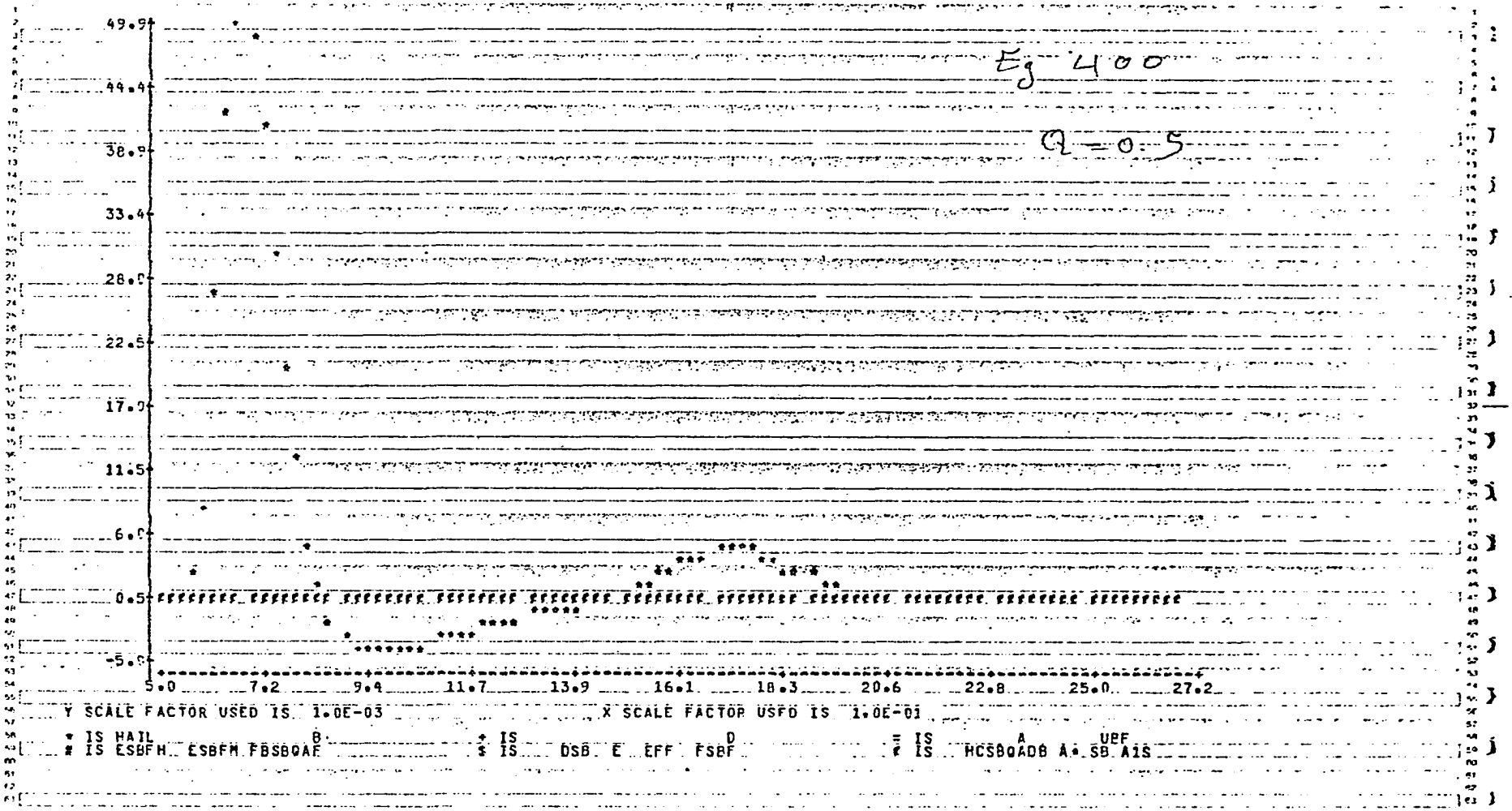
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6.0
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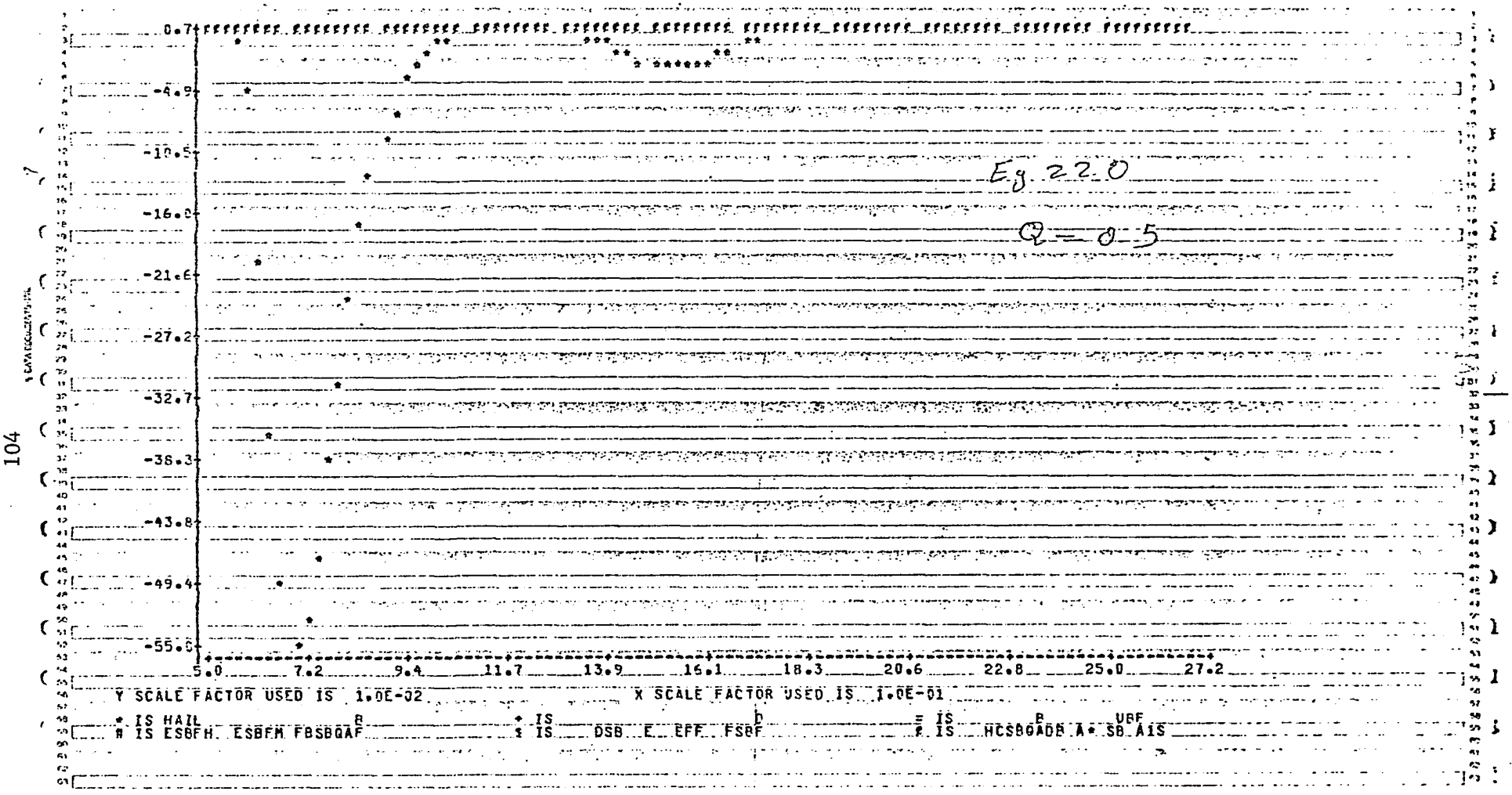
5.0
7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Y SCALE FACTOR USED IS 1.0E-03
X SCALE FACTOR USED IS 1.0E-01
* IS HAIL B + IS D = IS A UBF
# IS ESBFH ESBFM FBSBQAF $ IS DSB E EFF FSBF ¢ IS HCSBQADB A SB AIS

E_g $\theta = 0.5$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7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Eg. 22.0
Q = 0.5
Y SCALE FACTOR USED IS 1.0E-02
X SCALE FACTOR USED IS 1.0E-01
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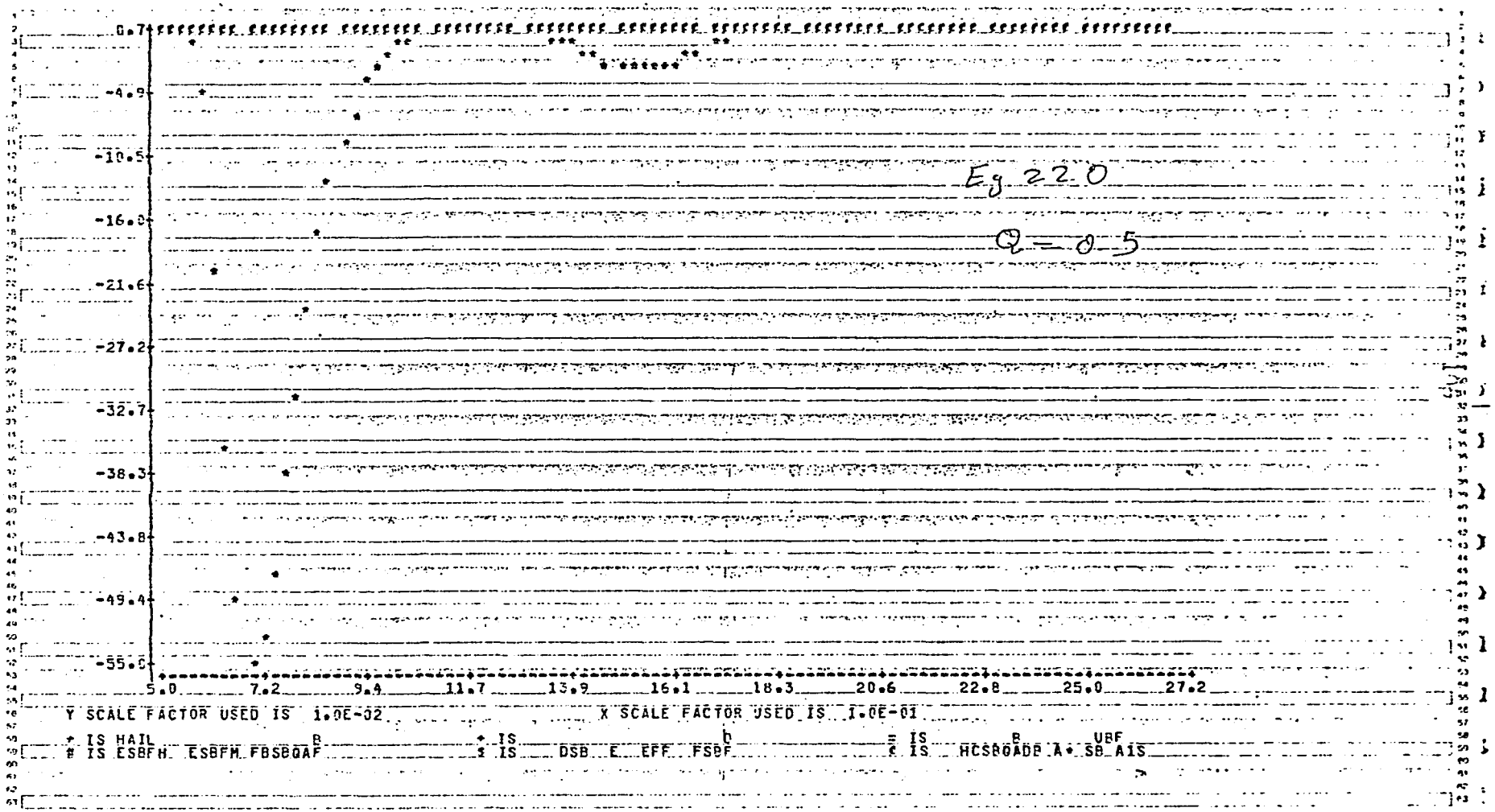
# IS ESBFH. ESBFM FBSBQAF
+ IS
$ IS DSB E EFF FSBF
= IS
% IS HCSBQADB A+ SB AIS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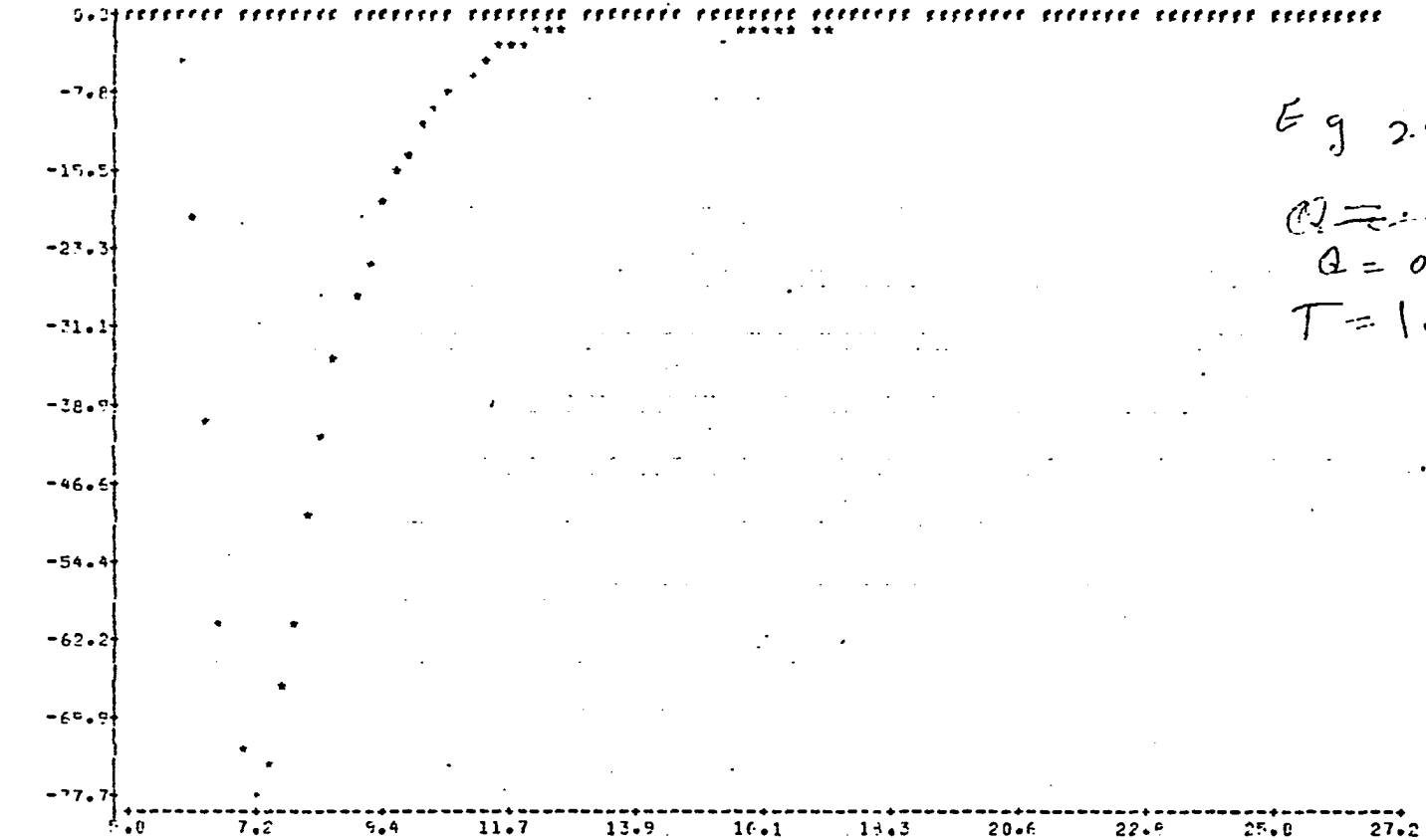
5.0
7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Y SCALE FACTOR USED IS 1.0E-02
X SCALE FACTOR USED IS 1.0E-01
* IS HAIL
# IS ESBFH ESBFM FBSBQAF
+ IS
I IS DSB E EFF FSBF
= IS
C IS HCSBQADB A SB AIS
UBF

Ej — a = 0.5



Eg 2.2.2.

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Q = 0.5

T = 1.277

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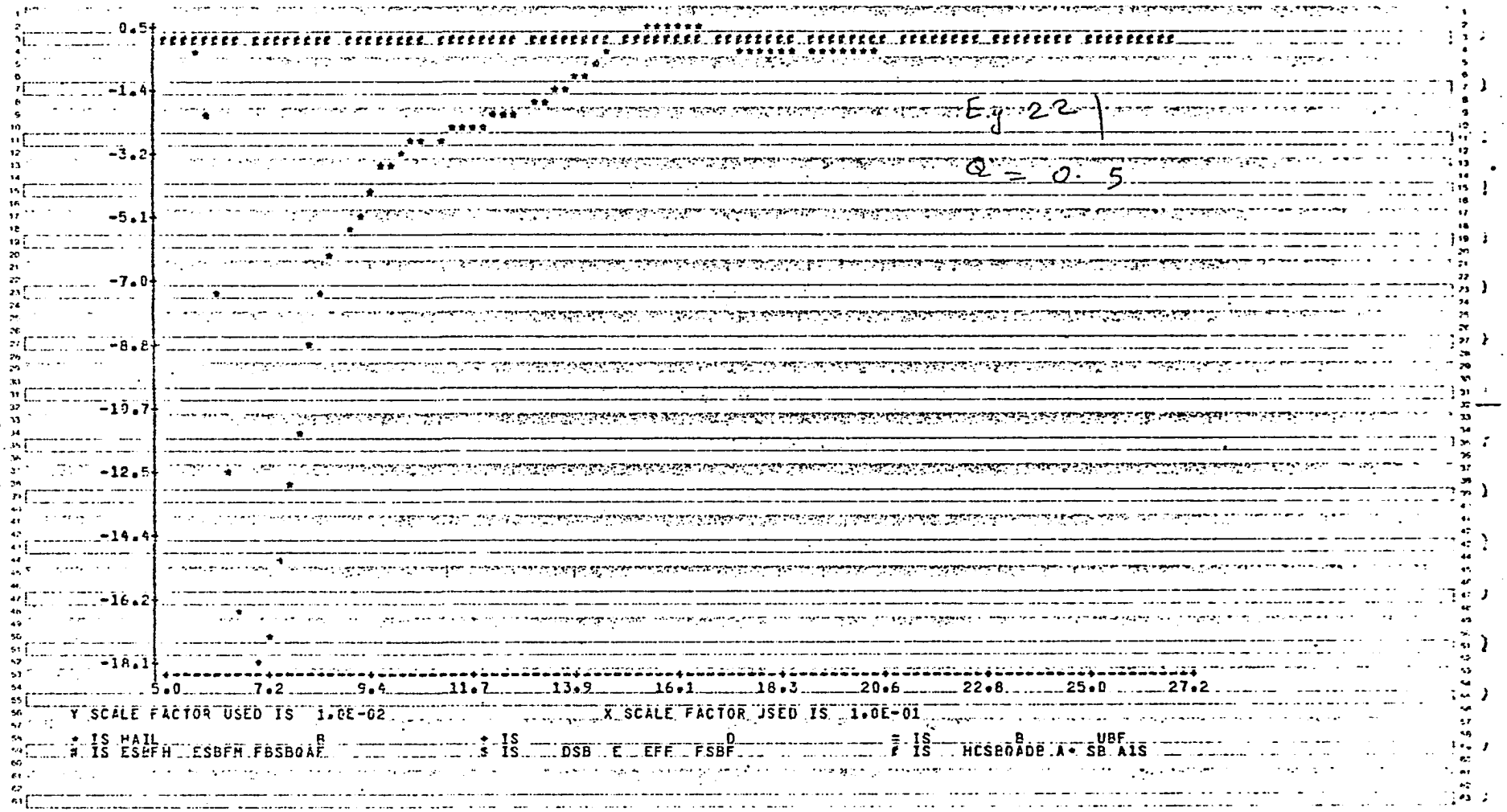
3	0.850	.0	.10515	.0	-.40932
4	0.875	.0	.93870E-01	.0	-.31897
5	0.900	-.5210493E-02	.66956E-01	.28250E-01	-.27149
6	0.925	-.2150230E-01	.61234E-01	.13500	-.24051
7	0.950	-.7535678E-01	.74892E-01	.59123	-.20235
8	0.975	-.1274591	.69317E-01	1.1880	-.17659
9	1.000	-.1681322	.63911E-01	1.8460	-.15495
10	1.025	-.1808456	.58583E-01	2.3174	-.13662
11	1.050	-.1741442	.53284E-01	2.5736	-.12095
12	1.075	-.1547665	.47956E-01	2.6013	-.10746
13	1.100	-.1316877	.42579E-01	2.4757	-.95770E-01
14	1.125	-.1163211	.37173E-01	2.3090	-.87550E-01
15	1.150	-.9164649E-01	.31774E-01	2.0377	-.76750E-01
16	1.175	-.7690269E-01	.26455E-01	1.8088	-.68970E-01
17	1.200	-.6523174E-01	.21274E-01	1.5970	-.62120E-01
18	1.225	-.5643334E-01	.16277E-01	1.4182	-.56070E-01
19	1.250	-.5464228E-01	.11488E-01	1.3230	-.52790E-01
20	1.275	-.4407377E-01	.69980E-02	1.1309	-.45970E-01
21	1.300	-.3979968E-01	.27432E-02	1.0262	-.41750E-01
22	1.325	-.3763978E-01	-.12475E-02	.94700	-.38710E-01
23	1.350	-.3414726E-01	-.49234E-02	.86732	-.34630E-01
24	1.375	-.3216664E-01	-.82772E-02	.80644	-.31610E-01
25	1.400	-.3044155E-01	-.11261E-01	.75800	-.28090E-01
26	1.425	-.2893174E-01	-.13842E-01	.71787	-.26460E-01
27	1.450	-.2672134E-01	-.15969E-01	.69500	-.25120E-01
28	1.475	-.2685564E-01	-.17590E-01	.67417	-.22290E-01
29	1.500	-.2609245E-01	-.18704E-01	.66538	-.20510E-01
30	1.525	-.2544356E-01	-.19292E-01	.66100	-.19200E-01
31	1.550	-.2399799E-01	-.19338E-01	.65286	-.17420E-01
32	1.575	-.2269639E-01	-.18658E-01	.65535	-.16090E-01
33	1.600	-.2181139E-01	-.17861E-01	.66700	-.14670E-01
34	1.625	-.2060857E-01	-.16380E-01	.68354	-.13770E-01
35	1.650	-.1921166E-01	-.14451E-01	.69600	-.13150E-01
36	1.675	-.1752956E-01	-.12118E-01	.73199	-.11830E-01
37	1.700	-.1564528E-01	-.94051E-02	.76486	-.10590E-01
38	1.725	-.1344796E-01	-.65670E-02	.79400	-.10370E-01
39	1.750	-.1093623E-01	-.35220E-02	.83850	-.95200E-02
40	1.775	-.8197263E-02	-.45601E-03	.87803	-.86700E-02
41	1.800	-.5300470E-02	.24988E-02	.92000	-.82700E-02
42	1.825	-.2432995E-02	.51982E-02	.96478	-.77200E-02
43	1.850	.5865470E-04	.74691E-02	.99200	-.74100E-02
44	1.875	.2516355E-02	.91387E-02	1.0534	-.67500E-02
45	1.900	.4625940E-02	.10045E-01	1.0950	-.63100E-02
46	1.925	.4625458E-02	.10094E-01	1.1270	-.59900E-02
47	1.950	.4416477E-02	.93121E-02	1.1745	-.55500E-02
48	1.975	.3179385E-02	.78531E-02	1.2029	-.52100E-02
49	2.000	.1334605E-02	.59841E-02	1.2200	-.48300E-02
50	2.025	-.7268125E-03	.40253E-02	1.2298	-.46000E-02
51	2.050	-.2673785E-02	.22597E-02	1.2220	-.44300E-02
52	2.075	-.3896661E-02	.69856E-03	1.2268	-.40700E-02
53	2.100	-.4679199E-02	-.17206E-04	1.2163	-.38300E-02
54	2.125	-.5067386E-02	-.56229E-03	1.2030	-.36500E-02
55	2.150	-.5021699E-02	-.67524E-03	1.1719	-.34100E-02
56	2.175	-.4927751E-02	-.10667E-02	1.1428	-.32200E-02
57	2.200	-.4784457E-02	-.12626E-02	1.1120	-.30400E-02
58	2.225	-.4622508E-02	-.14223E-02	1.0770	-.28700E-02
59	2.250	-.4555546E-02	-.15392E-02	1.0560	-.27700E-02
60	2.275	-.4232395E-02	-.16094E-02	1.0127	-.25700E-02
61	2.300	-.3981721E-02	-.16182E-02	.98602	-.24300E-02
62	2.325	-.3746632E-02	-.15447E-02	.96700	-.23300E-02
63	2.350	-.3630912E-02	-.14313E-02	.96700	-.23300E-02
64	2.375	-.3501374E-02	-.12909E-02	.96700	-.23300E-02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7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Eg-22
Q = 0.5
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X SCALE FACTOR USED IS 1.0E-01

E_g $a = 0.5$

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3	0.850	0	.17473E-01	0	.21560E-01
4	0.875	0	.14297E-01	0	.17580E-01
5	0.900	.75609146E-03	.11944E-01	.28250E-01	.14820E-01
6	0.925	.30815515E-02	.10016E-01	.13500	.12810E-01
7	0.950	.10778030E-01	.80198E-02	.59123	.10210E-01
8	0.975	.17673186E-01	.64665E-02	1.1880	.84100E-02
9	1.000	.22297645E-01	.51688E-02	1.8460	.69100E-02
10	1.025	.22628830E-01	.41044E-02	2.3174	.56600E-02
11	1.050	.20182701E-01	.32120E-02	2.5736	.46300E-02
12	1.075	.16378811E-01	.24962E-02	2.6013	.35000E-02
13	1.100	.12394225E-01	.18963E-02	2.4757	.31100E-02
14	1.125	.94209343E-02	.14198E-02	2.3090	.26600E-02
15	1.150	.62826055E-02	.98323E-03	2.0377	.21000E-02
16	1.175	.42783548E-02	.63527E-03	1.8080	.17300E-02
17	1.200	.28251515E-02	.33904E-03	1.5979	.14300E-02
18	1.225	.17858548E-02	.79275E-04	1.4182	.11800E-02
19	1.250	.11614798E-02	-.16697E-03	1.3230	.10600E-02
20	1.275	.54125537E-03	-.34140E-03	1.1309	.82000E-03
21	1.300	.17066688E-03	-.51271E-03	1.0202	.68000E-03
22	1.325	-.77397105E-04	-.67173E-03	.94700	.59000E-03
23	1.350	-.25916361E-03	-.77022E-03	.86332	.47000E-03
24	1.375	-.36672995E-03	-.85475E-03	.80644	.40000E-03
25	1.400	-.43521838E-03	-.91417E-03	.75800	.34000E-03
26	1.425	-.47027325E-03	-.94519E-03	.71787	.29000E-03
27	1.450	-.52045615E-03	-.10046E-02	.69900	.26000E-03
28	1.475	-.52762685E-03	-.99263E-03	.67417	.21600E-03
29	1.500	-.55121905E-03	-.99841E-03	.66538	.17000E-03
30	1.525	-.56563275E-03	-.10057E-02	.66100	.15000E-03
31	1.550	-.55739525E-03	-.98377E-03	.65206	.13000E-03
32	1.575	-.55897905E-03	-.96295E-03	.65535	.11000E-03
33	1.600	-.56062785E-03	-.93052E-03	.66700	.90000E-04
34	1.625	-.55045545E-03	-.88530E-03	.68354	.80000E-04
35	1.650	-.52608815E-03	-.82588E-03	.69600	.70000E-04
36	1.675	-.50745765E-03	-.75326E-03	.73199	.60000E-04
37	1.700	-.47161275E-03	-.66666E-03	.76486	.50000E-04
38	1.725	-.42112755E-03	-.57035E-03	.79400	.40000E-04
39	1.750	-.35672155E-03	-.46543E-03	.83850	.40000E-04
40	1.775	-.27404215E-03	-.35211E-03	.87803	.40000E-04
41	1.800	-.19317545E-03	-.23997E-03	.92000	.30000E-04
42	1.825	-.10227695E-03	-.12581E-03	.96478	.20000E-04
43	1.850	-.12176695E-04	-.32275E-04	.99200	.20000E-04
44	1.875	.68147265E-04	.44690E-04	1.0534	.20000E-04
45	1.900	.12803225E-03	.97103E-04	1.0950	.20000E-04
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47	1.950	.15447635E-03	.12153E-03	1.1745	.10000E-04
48	1.975	.12875025E-03	.97033E-04	1.2029	.10000E-04
49	2.000	.82293275E-04	.57454E-04	1.2209	.10000E-04
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51	2.050	-.35526705E-04	-.37213E-04	1.2320	.10000E-04
52	2.075	-.70881675E-04	-.67779E-04	1.2268	.10000E-04
53	2.100	-.99488365E-04	-.91796E-04	1.2163	.10000E-04
54	2.125	-.11471095E-03	-.10535E-03	1.2030	.10000E-04
55	2.150	-.12807285E-03	-.10926E-03	1.1719	.0
56	2.175	-.12164255E-03	-.10645E-03	1.1428	.0
57	2.200	-.11313535E-03	-.10174E-03	1.1126	.0
58	2.225	-.10735525E-03	-.99674E-04	1.0770	.0
59	2.250	-.10036515E-03	-.94759E-04	1.0569	.0
60	2.275	-.83216675E-04	-.82174E-04	1.0127	.0
61	2.300	-.75611315E-04	-.76685E-04	.98602	.0
62	2.325	-.67571535E-04	-.69877E-04	.96700	.0
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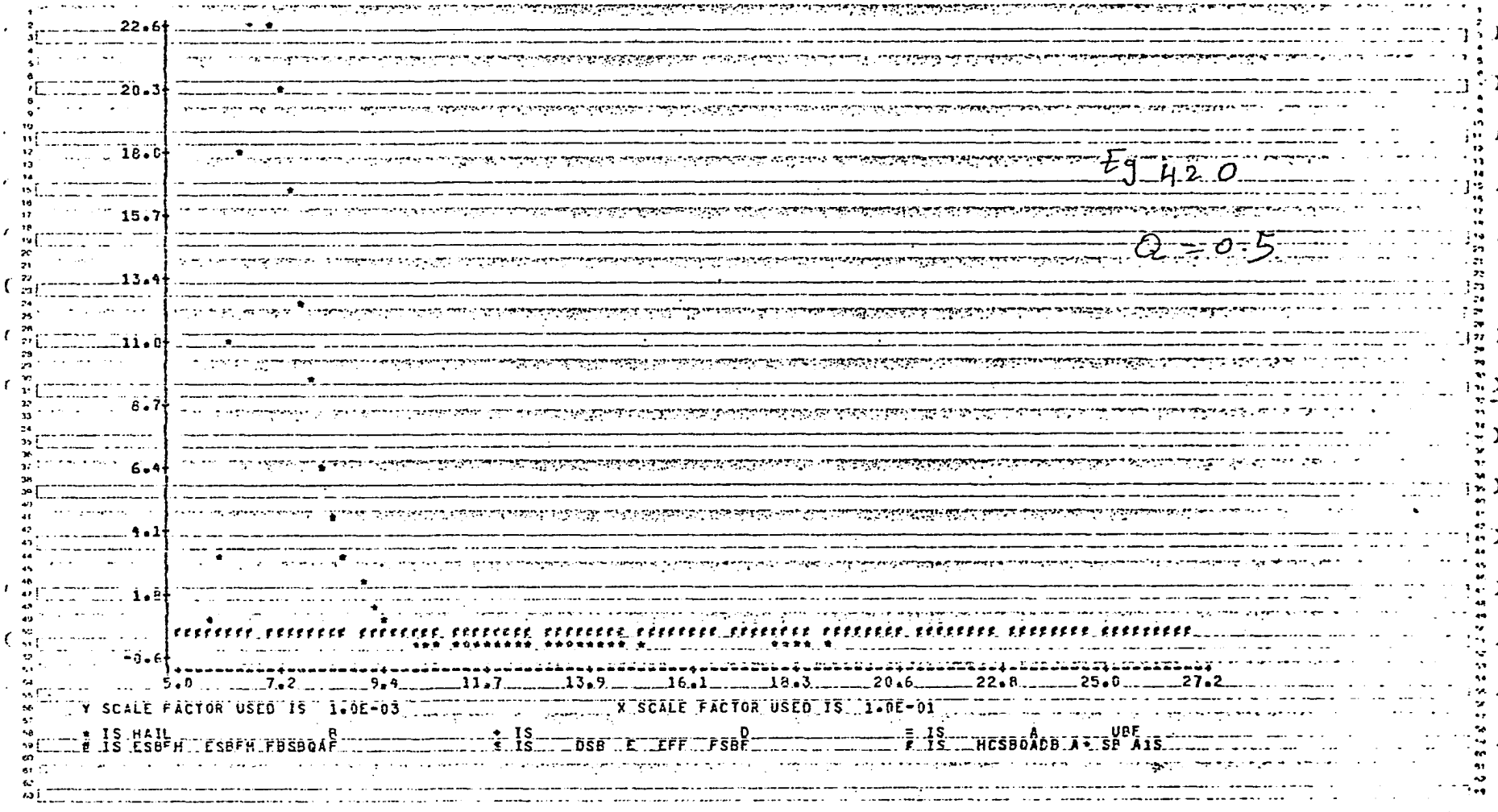
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13.4
11.0
8.7
6.4
4.1
1.8
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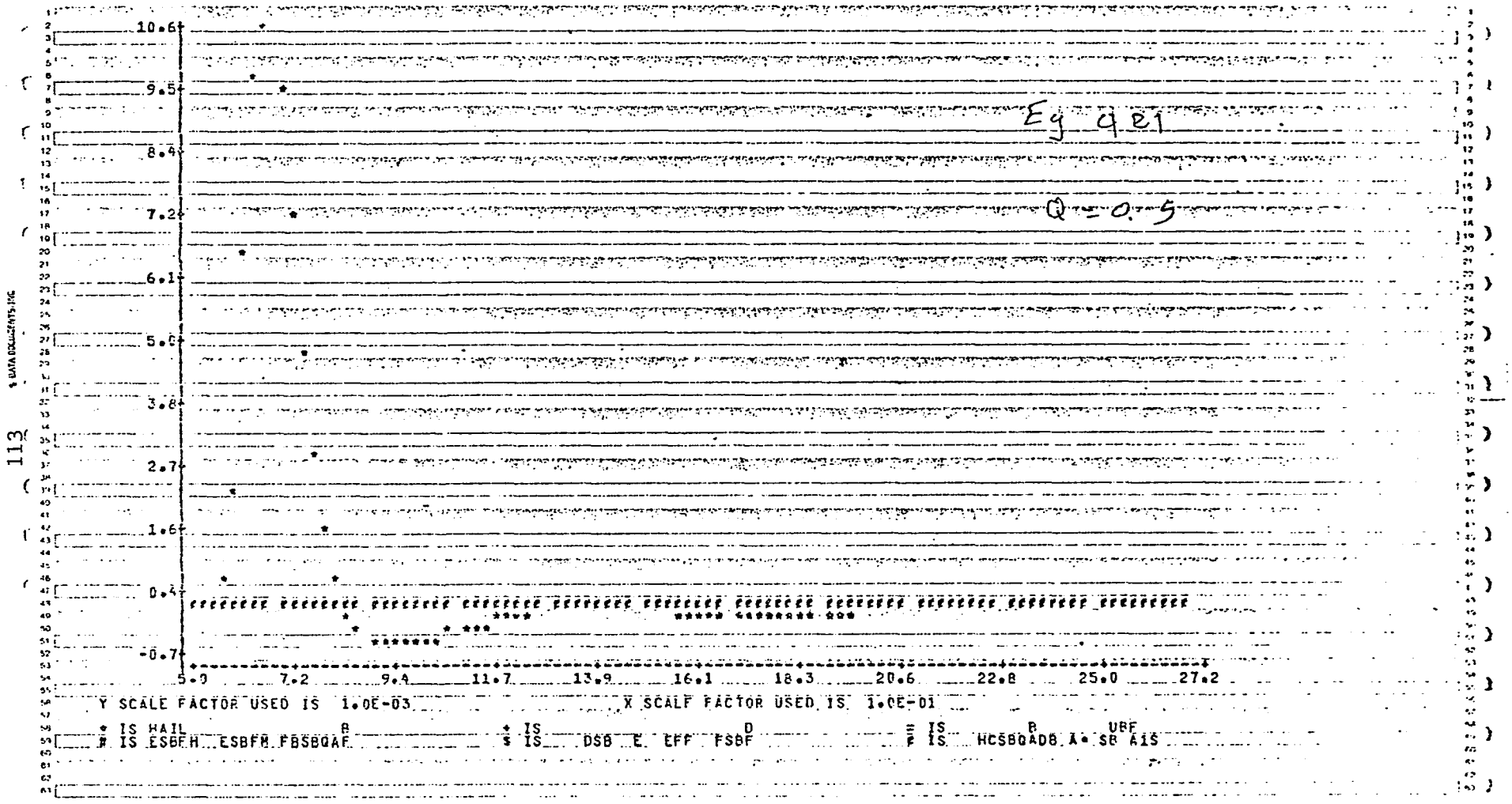
7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Eq 4.2.0
Q = 0.5
Y SCALE FACTOR USED IS 1.0E-03
X SCALE FACTOR USED IS 1.0E-01
* IS HAIL
B
* IS
D
= IS
A
UBF
E IS ESBFH ESBFH FBSBQAF
S IS DSB E EFF FSBF
F IS HCSBQADB A SB AIS

Eg 4 2 1

E.g. Q = 0.5

1	0.800	.0	.0	.0	.35090E-01
2	0.825	.0	.0	.0	.29690E-01
3	0.850	.0	.15247E-01	.0	.24290E-01
4	0.875	.0	.92878E-02	.0	.17670E-01
5	0.900	.5696204E-03	.60736E-02	.28250E-01	.14090E-01
6	0.925	.2124765E-02	.39590E-02	.13500	.11780E-01
7	0.950	.6524816E-02	.20266E-02	.59123	.90100E-02
8	0.975	.9537484E-02	.80826E-03	1.1080	.72200E-02
9	1.000	.1063366E-01	-.39605E-04	1.8460	.58000E-02
10	1.025	.9383220E-02	-.61102E-03	2.3174	.46600E-02
11	1.050	.7118437E-02	-.99403E-03	2.5736	.37600E-02
12	1.075	.4729766E-02	-.12218E-02	2.6013	.30400E-02
13	1.100	.2763347E-02	-.13538E-02	2.4757	.24700E-02
14	1.125	.1537546E-02	-.14241E-02	2.3090	.20900E-02
15	1.150	.4292438E-03	-.14293E-02	2.0377	.16400E-02
16	1.175	-.1413811E-03	-.14182E-02	1.8088	.13400E-02
17	1.200	-.4591080E-03	-.13675E-02	1.5970	.11000E-02
18	1.225	-.6153802E-03	-.13439E-02	1.4182	.91000E-03
19	1.250	-.6710929E-03	-.13173E-02	1.3230	.81000E-03
20	1.275	-.7163995E-03	-.12532E-02	1.1309	.62000E-03
21	1.300	-.6987229E-03	-.11949E-02	1.3202	.51000E-03
22	1.325	-.6588139E-03	-.11357E-02	.94700	.44000E-03
23	1.350	-.6013475E-03	-.10466E-02	.86332	.35000E-03
24	1.375	-.5264361E-03	-.95279E-03	.80644	.30000E-03
25	1.400	-.4567576E-03	-.85256E-03	.75800	.25000E-03
26	1.425	-.3947036E-03	-.75983E-03	.71787	.21000E-03
27	1.450	-.3305573E-03	-.66290E-03	.69900	.19000E-03
28	1.475	-.2621743E-03	-.53898E-03	.67417	.15000E-03
29	1.500	-.2018732E-03	-.43340E-03	.66538	.13000E-03
30	1.525	-.1502774E-03	-.33735E-03	.66100	.11000E-03
31	1.550	-.1010963E-03	-.24485E-03	.65286	.90000E-04
32	1.575	-.5409583E-04	-.16254E-03	.65535	.80000E-04
33	1.600	-.1343180E-04	-.90138E-04	.66700	.70000E-04
34	1.625	.2235660E-04	-.27293E-04	.68359	.60000E-04
35	1.650	.5314502E-04	.26358E-04	.69600	.50000E-04
36	1.675	.7831246E-04	.66986E-04	.73199	.40000E-04
37	1.700	.9409280E-04	.93020E-04	.76486	.30000E-04
38	1.725	.1090835E-03	.10738E-03	.79400	.30000E-04
39	1.750	.1152589E-03	.10746E-03	.83850	.30000E-04
40	1.775	.1007233E-03	.93826E-04	.87803	.30000E-04
41	1.800	.8436361E-04	.71696E-04	.92000	.20000E-04
42	1.825	.6915731E-04	.51630E-04	.96478	.20000E-04
43	1.850	.2816007E-04	.83872E-05	.99200	.20000E-04
44	1.875	-.2509962E-04	-.33826E-04	1.0539	.10000E-04
45	1.900	-.6658497E-04	-.70806E-04	1.0950	.10000E-04
46	1.925	-.1043691E-03	-.10260E-03	1.1270	.10000E-04
47	1.950	-.1371098E-03	-.12674E-03	1.1745	.10000E-04
48	1.975	-.1568176E-03	-.14203E-03	1.2029	.10000E-04
49	2.000	-.1682694E-03	-.14792E-03	1.2200	.10000E-04
50	2.025	-.1570388E-03	-.13767E-03	1.2298	.10000E-04
51	2.050	-.1599148E-03	-.13980E-03	1.2320	.10000E-04
52	2.075	-.1388623E-03	-.12319E-03	1.2268	.10000E-04
53	2.100	-.1186925E-03	-.10759E-03	1.2163	.10000E-04
54	2.125	-.1123861E-03	-.93421E-04	1.2030	.0
55	2.150	-.9414523E-04	-.80338E-04	1.1719	.0
56	2.175	-.7929525E-04	-.69389E-04	1.1428	.0
57	2.200	-.6518931E-04	-.56623E-04	1.1126	.0
58	2.225	-.4758014E-04	-.44176E-04	1.0770	.0
59	2.250	-.4453755E-04	-.42176E-04	1.0569	.0
60	2.275	-.3907757E-04	-.38580E-04	1.0127	.0
61	2.300	-.3296786E-04	-.33434E-04	.98602	.0
62	2.325	-.2961220E-04	-.30623E-04	.96700	.0
63	2.350	-.2703854E-04	-.27961E-04	.96700	.0
64	2.375	-.2457821E-04	-.25417E-04	.96700	.0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9.5
8.4
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3.8
2.7
1.6
0.4
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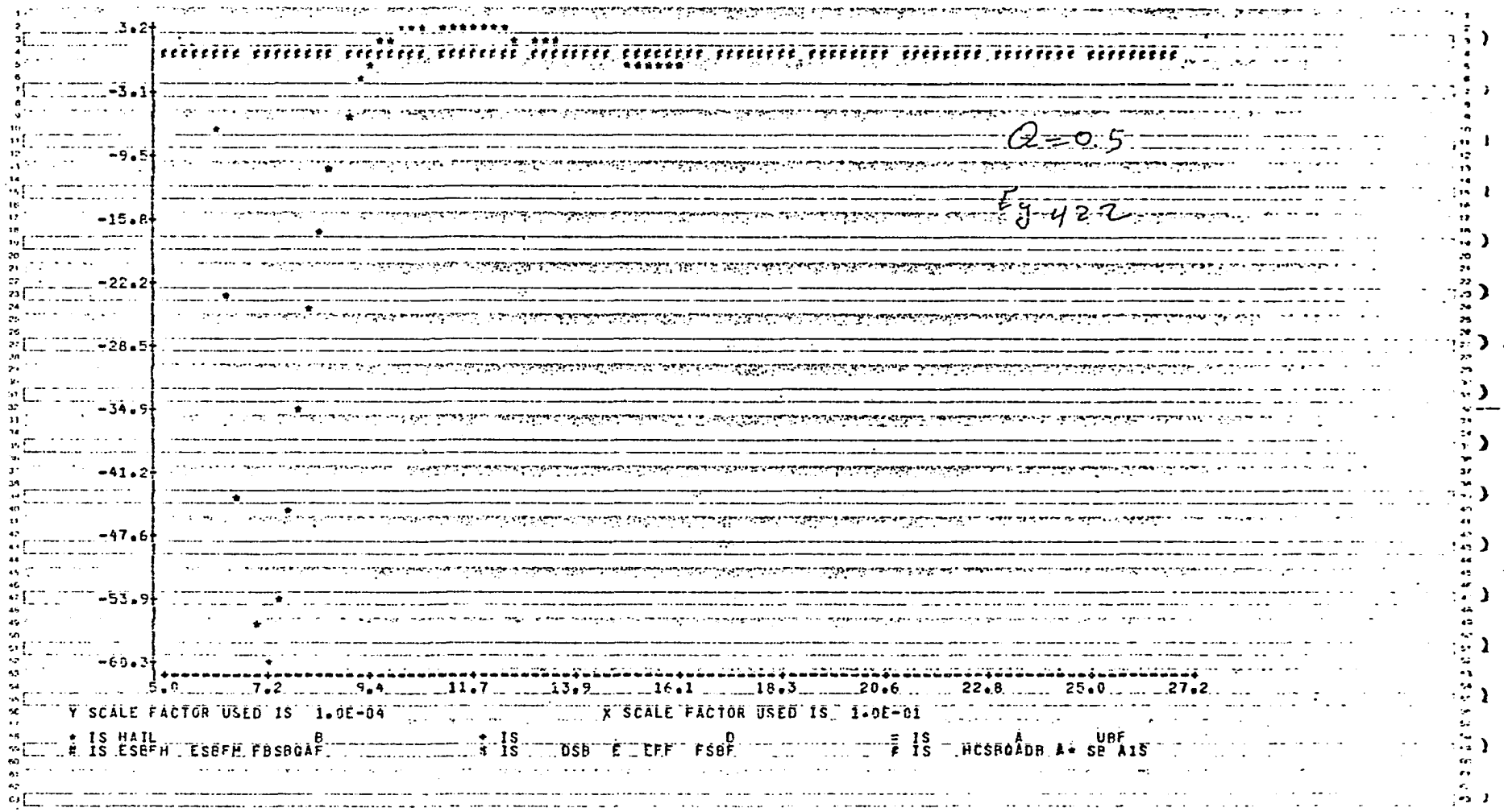
7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Eq 9.21
Q=0.5
Y SCALE FACTOR USED IS 1.0E-03
X SCALE FACTOR USED IS 1.0E-01
* IS HAIL B + IS D = IS B UBF
# IS ESBFH ESBFR FBSBQAF $ IS DSB E EFF FSBF ¢ IS HCSBQADB A SB AIS

E_y $Q = 0.5$

1	0.650	0	0	0	0	.61110E-01
2	0.625	0	0	0	0	.97760E-01
3	0.850	0	-.19189E-01	0	0	.34420E-01
4	0.875	0	-.15745E-01	0	0	.21820E-01
5	0.900	.6451318E-04	-.13416E-01	.28250E-01	.16100E-01	
6	0.925	.5396013E-04	-.12400E-01	.13500	.12800E-01	
7	0.950	.7980615E-03	-.10501E-01	.59123	.91500E-02	
8	0.975	.2455294E-02	-.97768E-02	1.1889	.70190E-02	
9	1.000	.4386653E-02	-.78012E-02	1.6460	.54290E-02	
10	1.025	.5657174E-02	-.66511E-02	2.3174	.42100E-02	
11	1.050	.6205545E-02	-.56413E-02	2.5736	.33000E-02	
12	1.075	.5492777E-02	-.47216E-02	2.6013	.26100E-02	
13	1.100	.4554249E-02	-.39095E-02	2.4757	.20700E-02	
14	1.125	.3516059E-02	-.32528E-02	2.3090	.17300E-02	
15	1.150	.2520076E-02	-.26675E-02	2.0477	.13300E-02	
16	1.175	.1726761E-02	-.20246E-02	1.8088	.10700E-02	
17	1.200	.1102185E-02	-.15602E-02	1.5970	.87300E-03	
18	1.225	.6552846E-03	-.11721E-02	1.4182	.71000E-03	
19	1.250	.2946018E-03	-.85260E-03	1.3230	.63000E-03	
20	1.275	.8868612E-04	-.59842E-03	1.1309	.48000E-03	
21	1.300	.7116983E-04	-.33022E-03	1.0202	.40000E-03	
22	1.325	.1847635E-03	-.14490E-03	.94700	.34000E-03	
23	1.350	.2377237E-03	.53564E-05	.86332	.27000E-03	
24	1.375	.2830567E-03	.12100E-03	.80644	.23000E-03	
25	1.400	.3020206E-03	.20845E-03	.75800	.19000E-03	
26	1.425	.3096738E-03	.26441E-03	.71787	.16000E-03	
27	1.450	.3213524E-03	.31973E-03	.69500	.14000E-03	
28	1.475	.2819508E-03	.32305E-03	.67417	.11300E-03	
29	1.500	.2745471E-03	.32262E-03	.66538	.10000E-04	
30	1.525	.2611509E-03	.31511E-03	.66100	.80000E-04	
31	1.550	.2242470E-03	.29348E-03	.65286	.60000E-04	
32	1.575	.2356236E-03	.25071E-03	.65535	.50000E-04	
33	1.600	.1746022E-03	.21177E-03	.66700	.50000E-04	
34	1.625	.1455576E-03	.17227E-03	.68354	.40000E-04	
35	1.650	.1127586E-03	.12201E-03	.69600	.40000E-04	
36	1.675	.8347916E-04	.84044E-04	.73199	.30000E-04	
37	1.700	.4732269E-04	.41845E-04	.76486	.20000E-04	
38	1.725	.2107950E-04	.6548E-05	.79400	.20000E-04	
39	1.750	-.6196211E-05	-.27782E-04	.83750	.20000E-04	
40	1.775	-.2933662E-04	-.53405E-04	.87803	.20000E-04	
41	1.800	-.4556671E-04	-.73227E-04	.92000	.20000E-04	
42	1.825	-.5610267E-04	-.78516E-04	.96478	.10000E-04	
43	1.850	-.6114024E-04	-.81795E-04	.99200	.10000E-04	
44	1.875	-.6731667E-04	-.92087E-04	1.0534	.10000E-04	
45	1.900	-.8298168E-04	-.95789E-04	1.0850	.10000E-04	
46	1.925	-.7271391E-04	-.74520E-04	1.1270	.10000E-04	
47	1.950	-.6091239E-04	-.61915E-04	1.1745	.10000E-04	
48	1.975	-.4763110E-04	-.49597E-04	1.2029	.10000E-04	
49	2.000	-.3473376E-04	-.36519E-04	1.2200	.10000E-04	
50	2.025	-.4246214E-04	-.34528E-04	1.2298	.0	
51	2.050	-.3246610E-04	-.26369E-04	1.2320	.0	
52	2.075	-.2511885E-04	-.20467E-04	1.2268	.0	
53	2.100	-.2068219E-04	-.21471E-04	1.2163	.0	
54	2.125	-.2329918E-04	-.19360E-04	1.2030	.0	
55	2.150	-.2035624E-04	-.20812E-04	1.1719	.0	
56	2.175	-.2137777E-04	-.18757E-04	1.1428	.0	
57	2.200	-.1664934E-04	-.16771E-04	1.1120	.0	
58	2.225	-.1603254E-04	-.14906E-04	1.0770	.0	
59	2.250	-.1584453E-04	-.15014E-04	1.0569	.0	
60	2.275	-.1163677E-04	-.11392E-04	1.0127	.0	
61	2.300	-.1162675E-04	-.11792E-04	.98602	.0	
62	2.325	-.9872506E-05	-.10209E-04	.96700	.0	
63	2.350	-.1021867E-04	-.10567E-04	.96700	.0	
64	2.375	-.8648839E-05	-.89812E-05	.96700	.0	


3.2
-3.1
-9.5
-15.8
-22.2
-28.5
-34.9
-41.2
-47.6
-53.9
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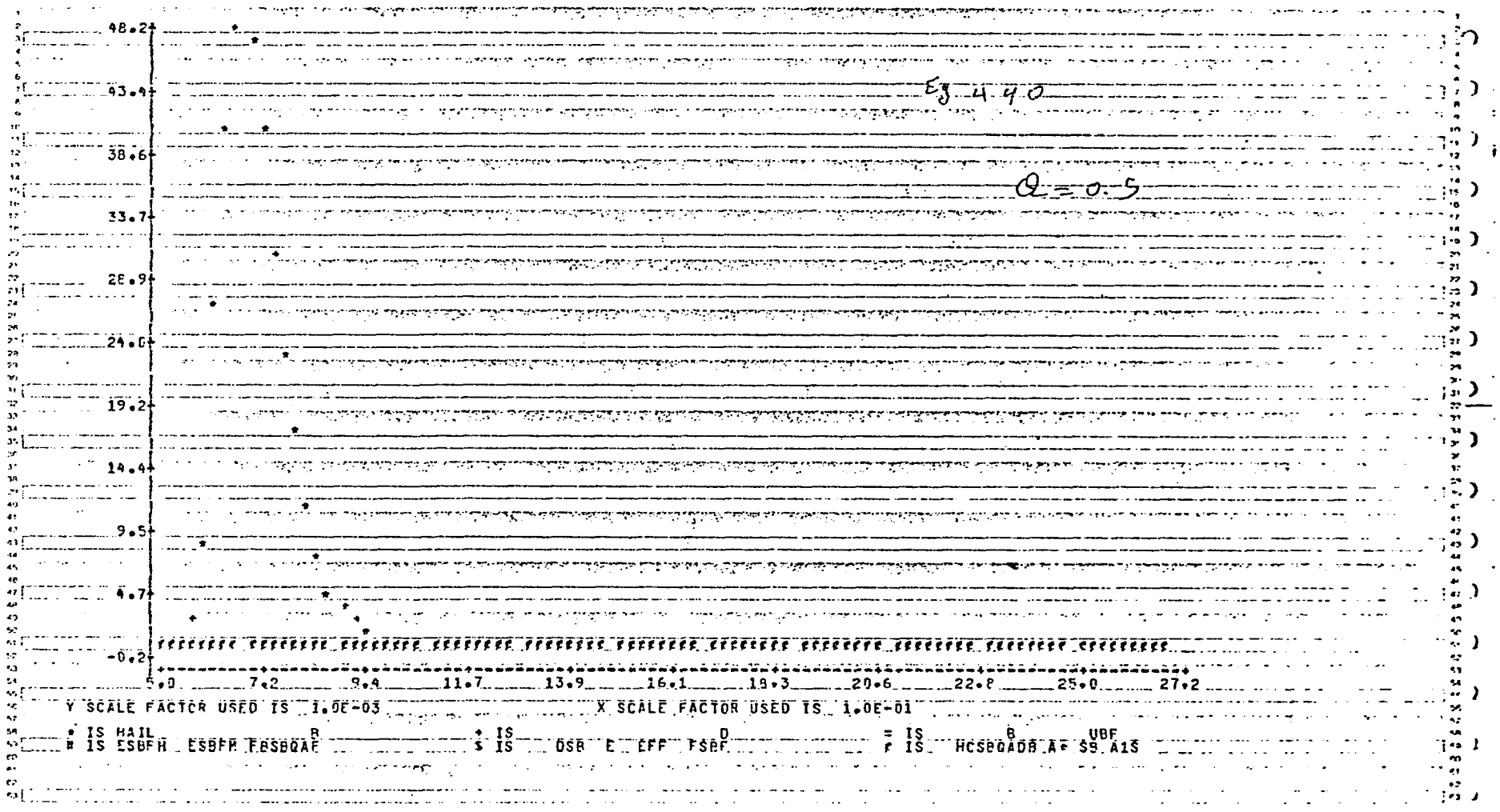
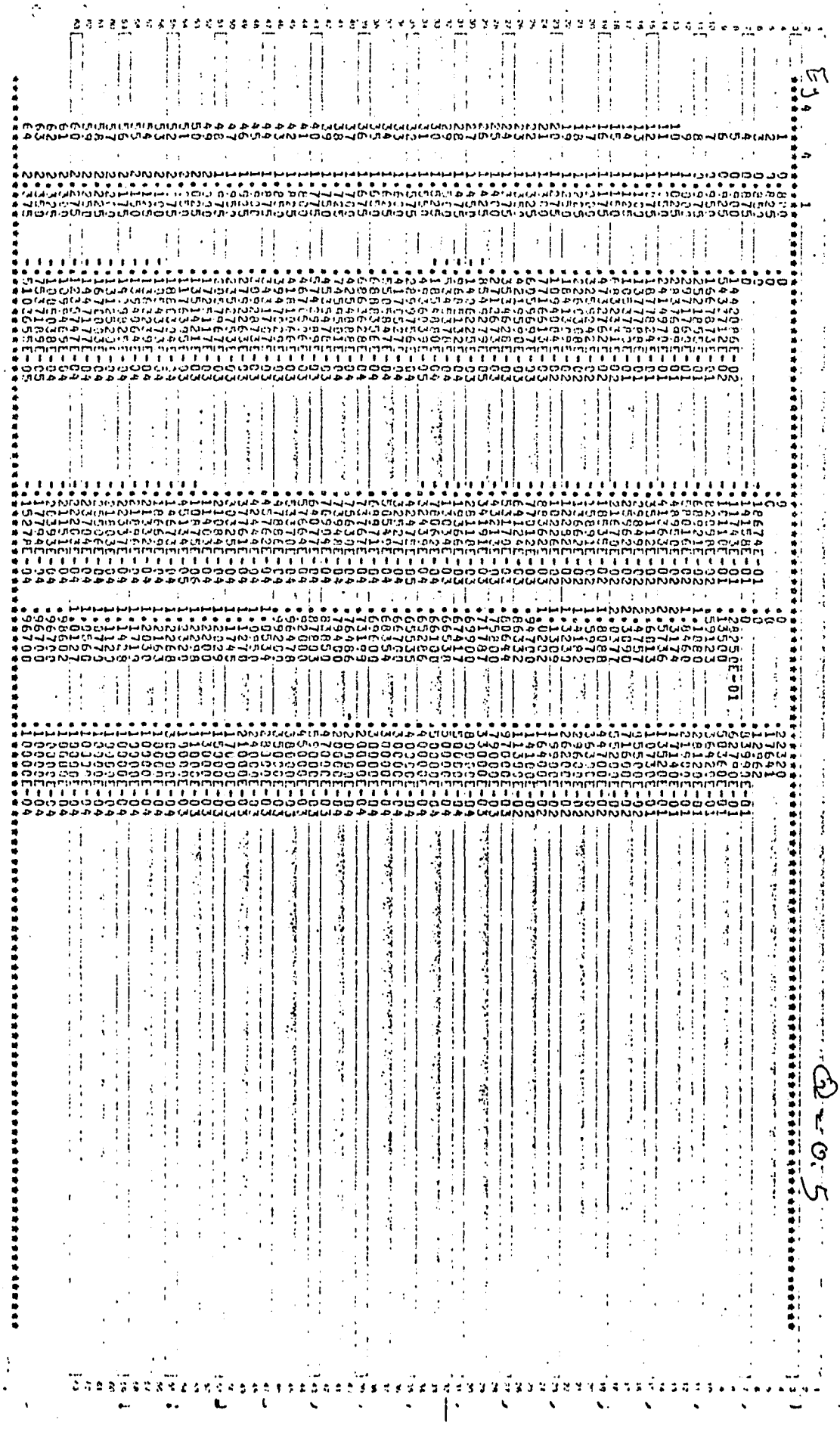
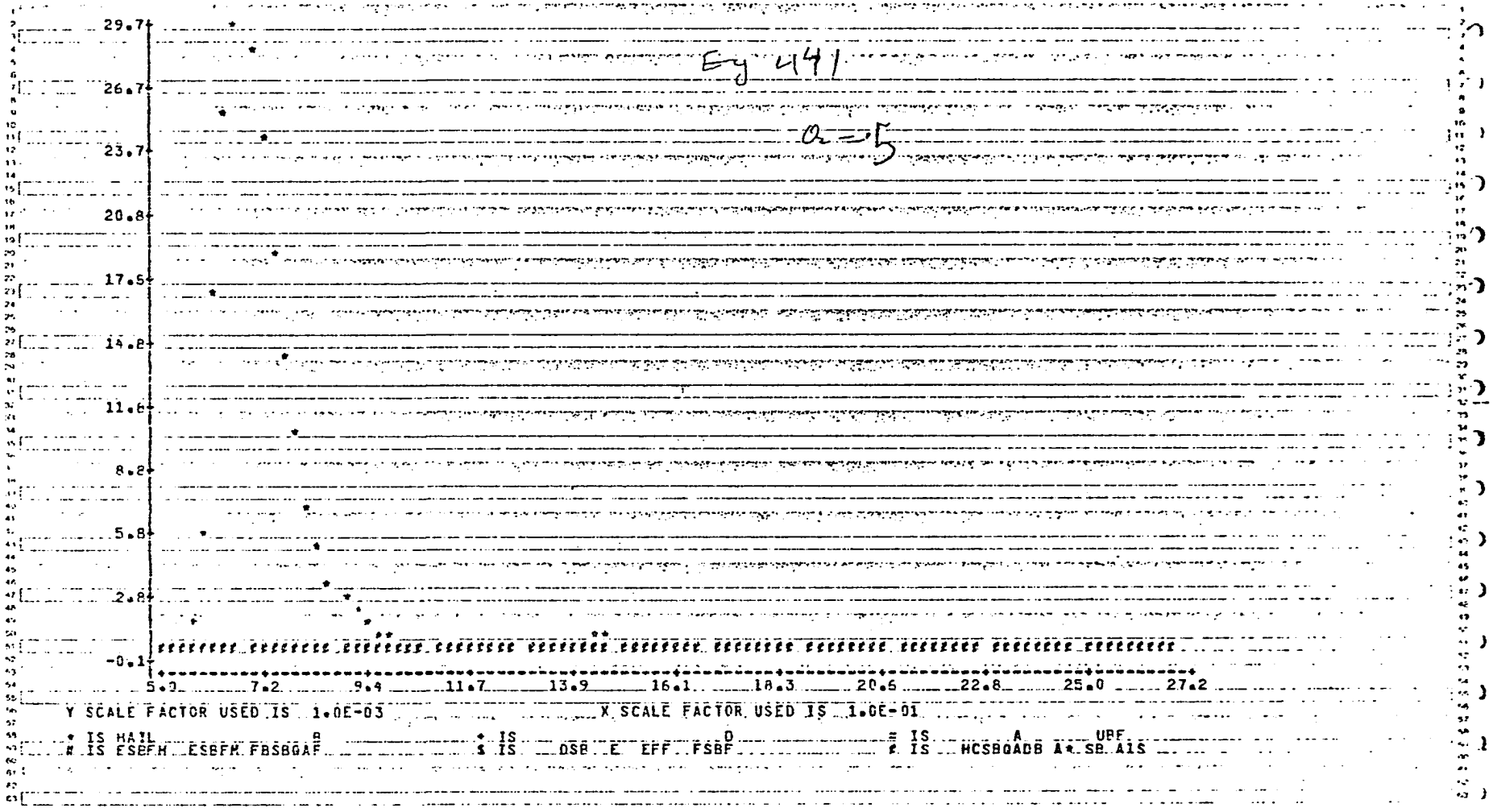
5.0
7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Q=0.5
Eg-42
Y SCALE FACTOR USED IS 1.0E-04
X SCALE FACTOR USED IS 1.0E-01
* IS HAIL B * IS D = IS A UBF
# IS ESBFH ESBFH FBSBOAF $ IS DSB E EFF FSBF ? IS HCSBOADB A* SB A1S

E3
E4 Q=0.5


48.2
43.4
38.6
33.7
28.9
24.0
19.2
14.4
9.5
4.7
-0.2
5.0
7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Eg 4.40
Q = 0.5
Y SCALE FACTOR USED IS 1.0E-03
X SCALE FACTOR USED IS 1.0E-01
* IS HAIL
# IS ESBFH ESBFM FESBQAF B
+ IS
$ IS OSB E EFF FSBF D
= IS B UBF
F IS HCSBQADB AF S9 A1S




Eq 441
a=5
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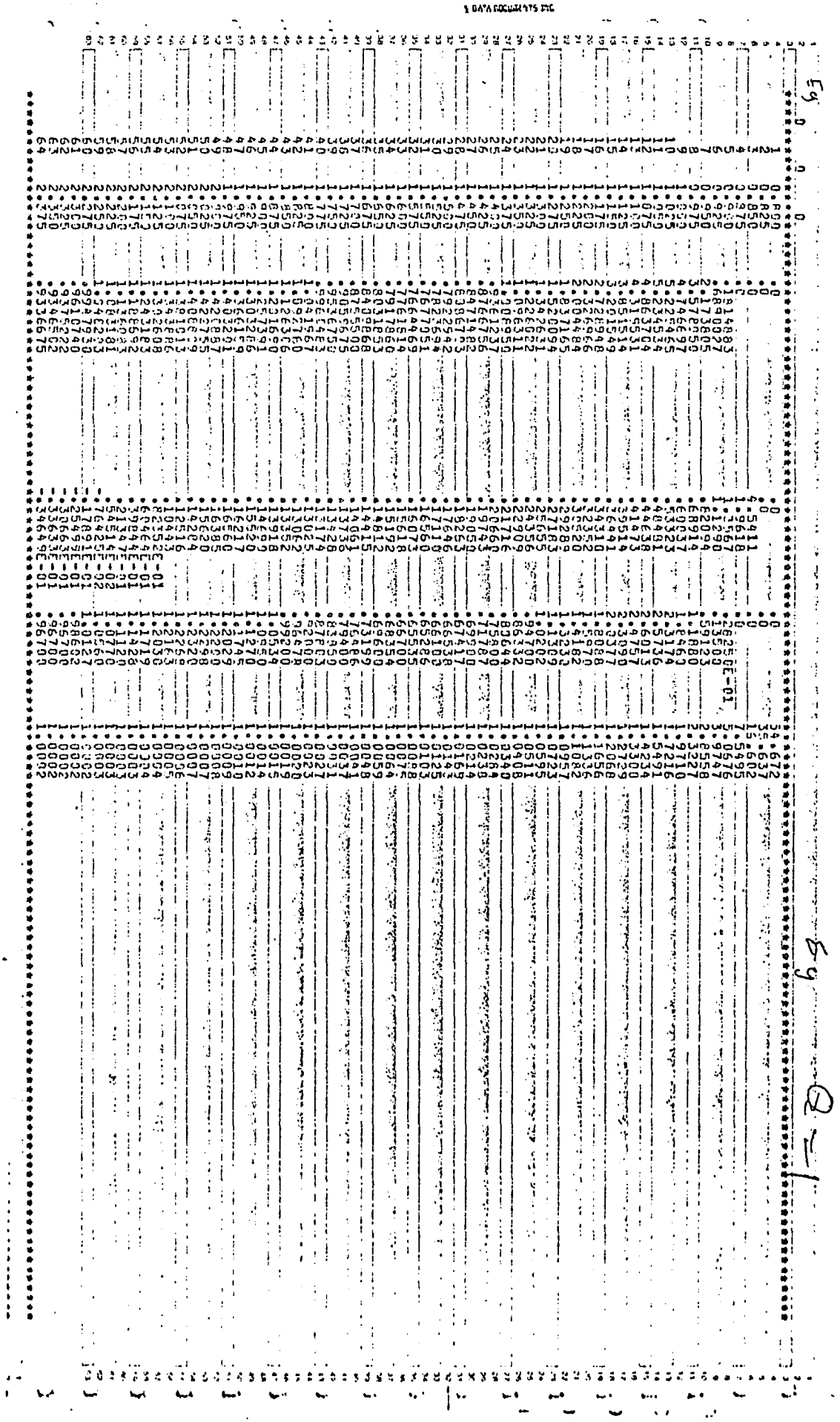
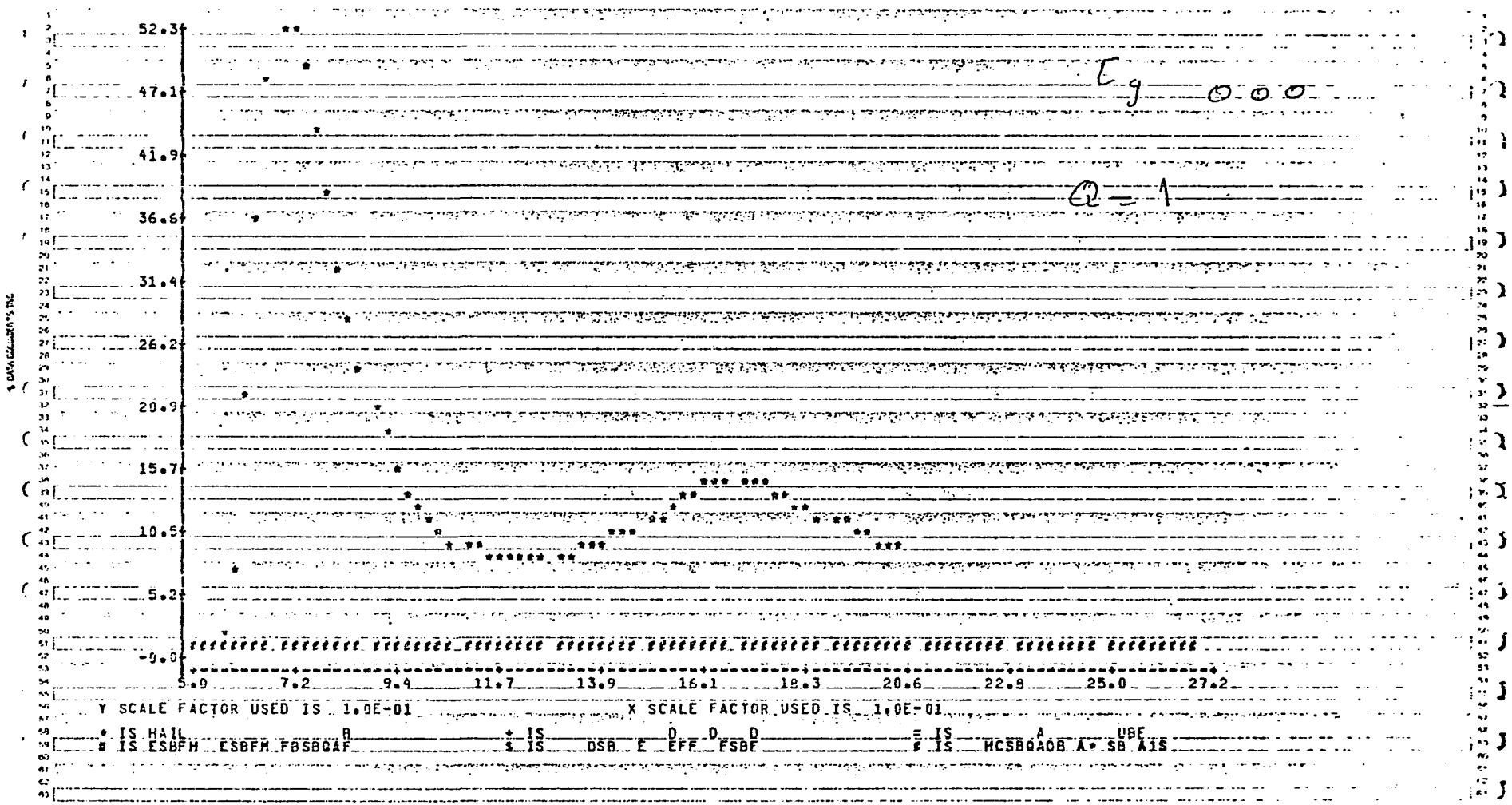
26.7
23.7
20.8
17.5
14.8
11.6
8.2
5.8
2.8
-0.1
5.0
7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Y SCALE FACTOR USED IS 1.0E-03
X SCALE FACTOR USED IS 1.0E-01
* IS HAIL
# IS ESBFH ESBFM FBSBOAF
B
+ IS
$ IS DSB E EFF FSBF
D
= IS
@ IS HCSBOADB A* SB AIS
A
UBF




52.3
47.1
41.9
36.6
31.4
26.2
20.9
15.7
10.5
5.2
-0.0
5.0
7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Eg 0.00
Q = 1
Y SCALE FACTOR USED IS 1.0E-01
X SCALE FACTOR USED IS 1.0E-01

Eg 2 0 0 — Eg — Q = 1

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2	0.825	.0	.0	.0	12.786	
3	0.850	.0	-2.1559	.0	5.5120	
4	0.875	.0	-.48147	.0	2.2202	
5	0.900	.3673251E-01	-.63954E-01	.28250E-01	1.3642	
6	0.925	.1524877	.13196	.13500	.99758	
7	0.950	.4743767	.18008	.59123	.62228	
8	0.975	.7783252	.20811	1.1880	.44705	
9	1.000	1.014278	.21748	1.8460	.33197	
10	1.025	1.079761	.21577	2.3174	.25016	
11	1.050	1.042187	.21160	2.5736	.19336	
12	1.075	.9280614	.20524	2.6013	.15153	
13	1.100	.7871059	.19783	2.4757	.12010	
14	1.125	.6796374	.19373	2.3090	.10061	
15	1.150	.5294652	.18166	2.0377	.77690E-01	
16	1.175	.4268564	.17284	1.8088	.63150E-01	
17	1.200	.3435683	.16348	1.5970	.51650E-01	
18	1.225	.2777723	.15346	1.4182	.42410E-01	
19	1.250	.2409132	.14431	1.3230	.37790E-01	
20	1.275	.1814546	.13145	1.1509	.29000E-01	
21	1.300	.1466104	.11960	1.0202	.24110E-01	
22	1.325	.1216736	.10762	.94700	.20860E-01	
23	1.350	.9660077E-01	.9806SE-01	.86332	.16830E-01	
24	1.375	.7824183E-01	.82891E-01	.80644	.14130E-01	
25	1.400	.6295848E-01	.71169E-01	.75000	.11890E-01	
26	1.425	.5037577E-01	.60134E-01	.71787	.10040E-01	
27	1.450	.4133392E-01	.50019E-01	.69900	.90800E-02	
28	1.475	.3220016E-01	.40563E-01	.67417	.72000E-02	
29	1.500	.2541039E-01	.32069E-01	.66538	.61200E-02	
30	1.525	.1977742E-01	.24538E-01	.66100	.53900E-02	
31	1.550	.1455813E-01	.17839E-01	.65286	.44690E-02	
32	1.575	.1051810E-01	.12230E-01	.65535	.38200E-02	
33	1.600	.7330211E-02	.77310E-02	.66700	.32700E-02	
34	1.625	.4937876E-02	.44140E-02	.68354	.28100E-02	
35	1.650	.3522220E-02	.24907E-02	.69600	.25700E-02	
36	1.675	.2619754E-02	.14289E-02	.73199	.20900E-02	
37	1.700	.2796669E-02	.18464E-02	.76486	.18100E-02	
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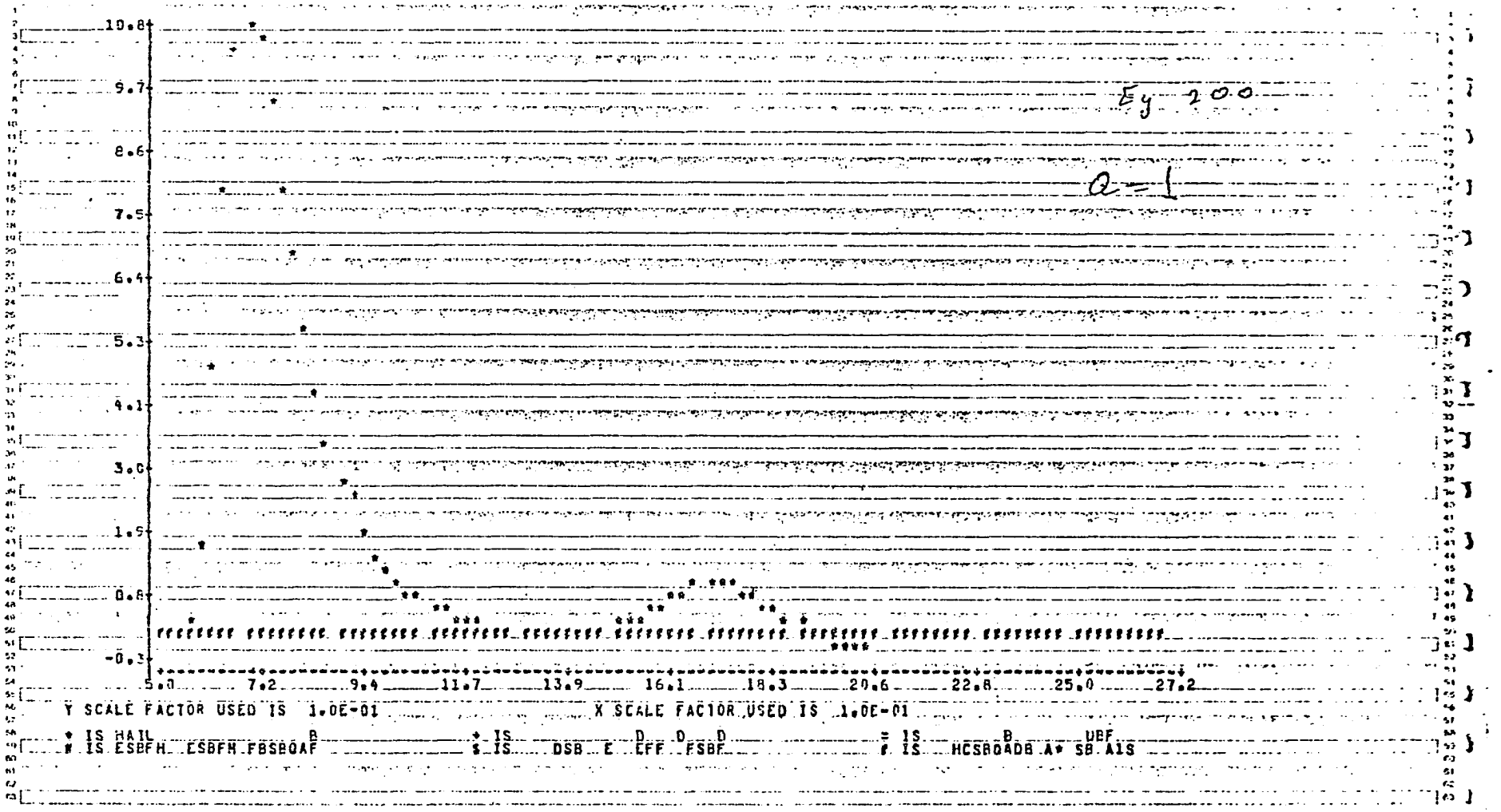
39	1.750	.6055441E-02	.58518E-02	.83859	.13700E-02	
40	1.775	.9202573E-02	.93009E-02	.87803	.11800E-02	
41	1.800	.1363355E-01	.13789E-01	.92000	.10300E-02	
42	1.825	.1968719E-01	.19509E-01	.96478	.90000E-03	
43	1.850	.2728796E-01	.26678E-01	.99200	.83000E-03	
44	1.875	.3716005E-01	.34585E-01	1.0534	.69000E-03	
45	1.900	.4792126E-01	.43152E-01	1.0950	.61000E-03	
46	1.925	.5873226E-01	.51564E-01	1.1270	.55000E-03	
47	1.950	.6978422E-01	.58996E-01	1.1745	.47000E-03	
48	1.975	.7856363E-01	.64892E-01	1.2029	.42000E-03	
49	2.000	.8447242E-01	.68870E-01	1.2200	.37000E-03	
50	2.025	.8722180E-01	.70605E-01	1.2298	.32000E-03	
51	2.050	.8669192E-01	.70067E-01	1.2320	.30000E-03	
52	2.075	.8262038E-01	.67087E-01	1.2268	.26000E-03	
53	2.100	.7554460E-01	.61092E-01	1.2163	.22000E-03	
54	2.125	.6600288E-01	.54666E-01	1.2030	.20000E-03	
55	2.150	.5386151E-01	.45782E-01	1.1719	.18000E-03	
56	2.175	.4115411E-01	.35088E-01	1.1420	.16000E-03	
57	2.200	.2861693E-01	.25995E-01	1.1120	.14000E-03	
58	2.225	.1675814E-01	.15430E-01	1.0770	.13000E-03	
59	2.250	.6204031E-02	.5755OE-02	1.0560	.12000E-03	
60	2.275	-.3167671E-02	-.3228OE-02	1.0127	.10000E-03	
61	2.300	-.1106415E-01	-.11311E-01	.98602	.90000E-04	
62	2.325	-.1774757E-01	-.18433E-01	.96700	.80000E-04	
63	2.350	-.2365409E-01	-.24541E-01	.96700	.80000E-04	
64	2.375	-.2856939E-01	-.29624E-01	.96700	.80000E-04	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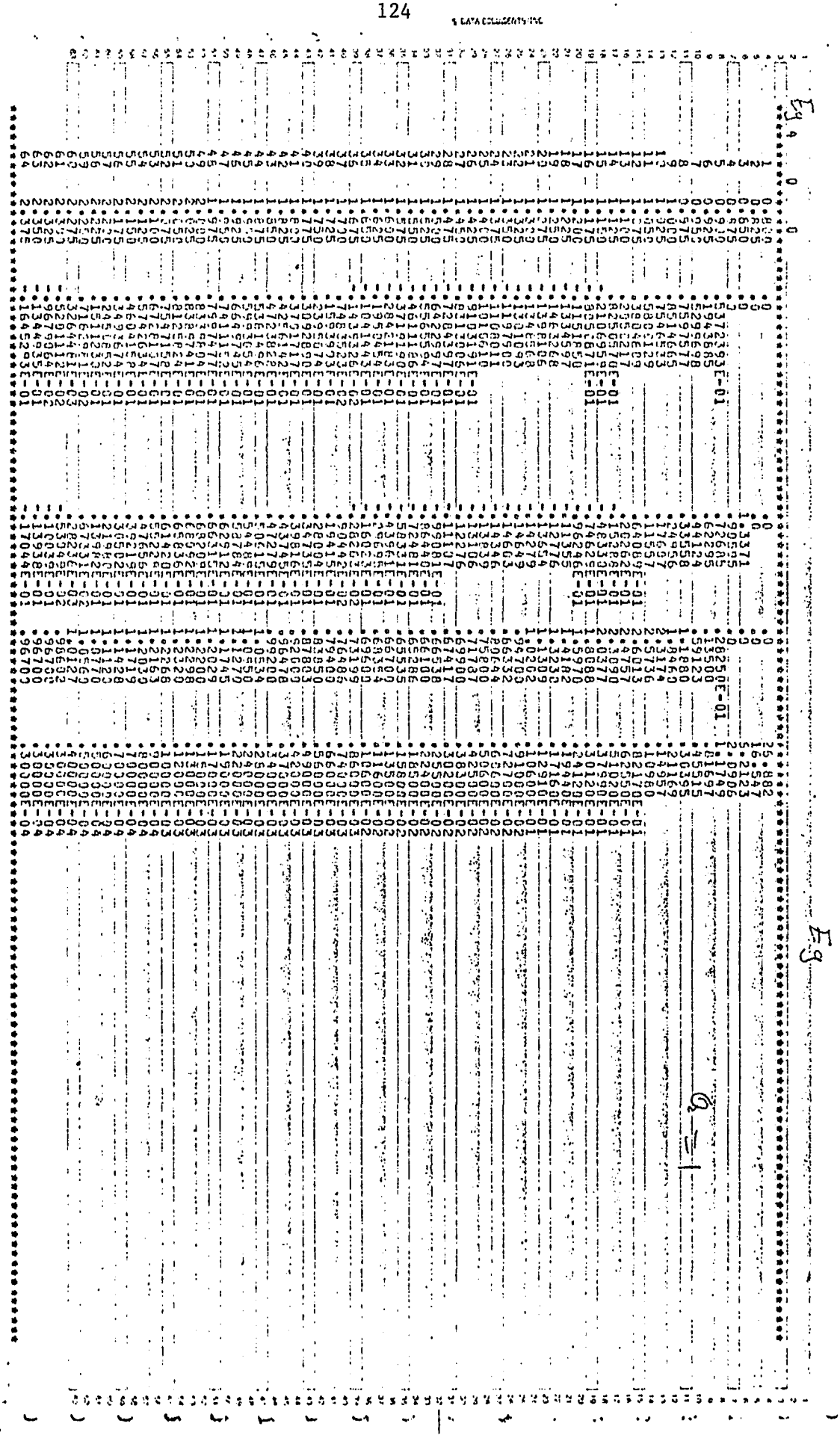
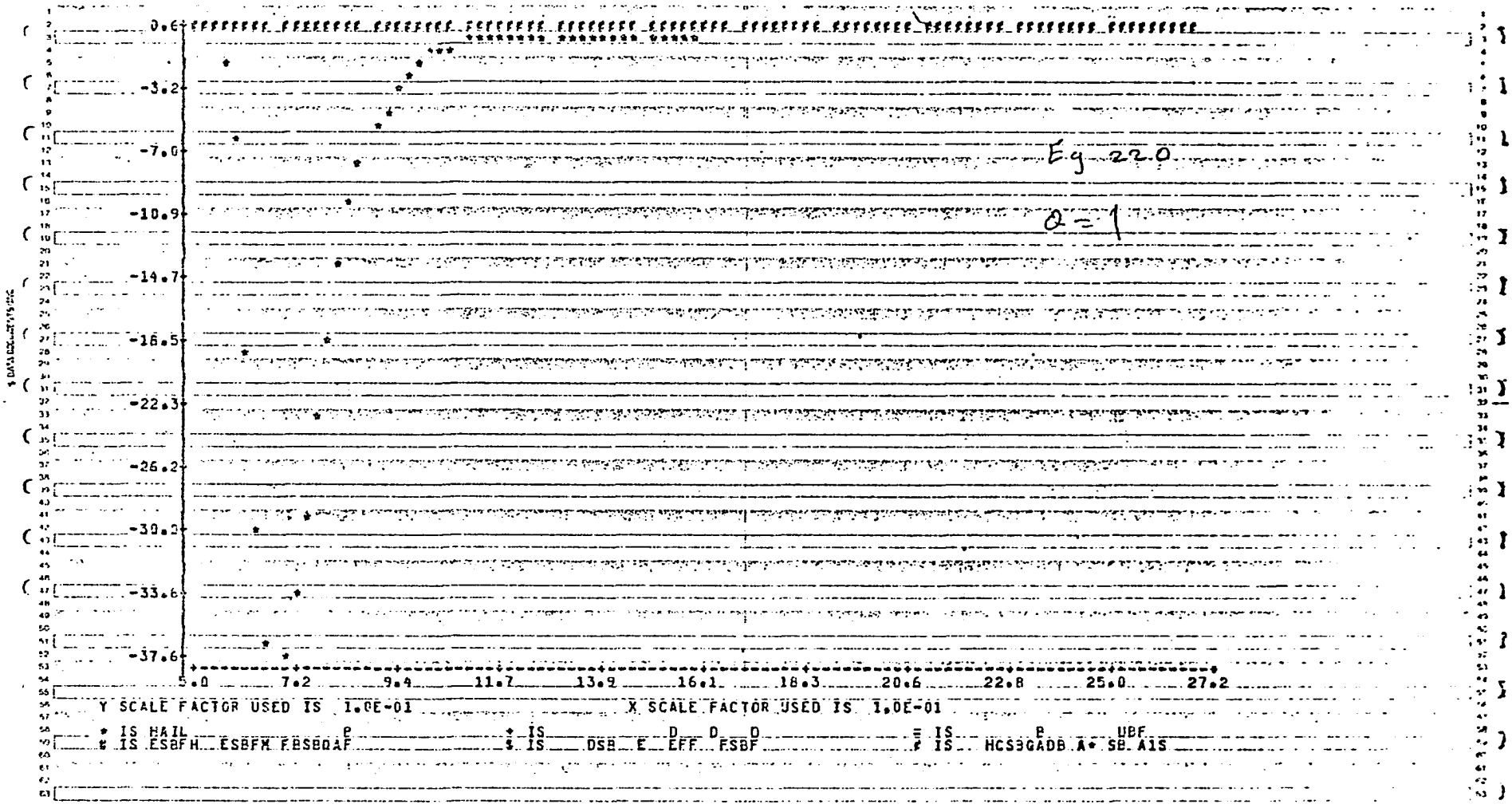
7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Ey 200
Q=1
Y SCALE FACTOR USED IS 1.0E-01
X SCALE FACTOR USED IS 1.0E-01
* IS HAIL B
# IS ESBFH ESBFH FBSBQAF
+ IS D D D
$ IS DSB E EFF FSBF
= IS B UBF
@ IS HCSBQADB A* SB A1S



65.1
75.2
65.2
55.2
45.2
35.3
25.3
15.3
5.3
-4.7
-14.6
5.0
7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Eg 400
a = 1
Y SCALE FACTOR USED IS 1.0E-02
X SCALE FACTOR USED IS 1.0E-01

Eq 2 2 0 Eq 2 = 1

1	0.800	.0	.0	.0	-59.408	
2	0.825	.0	.0	.0	-44.241	
3	0.850	.0	-4.6764	.0	-19.074	
4	0.875	.0	-2.2629	.0	-7.8031	
5	0.900	-.1837766	-1.6068	.28250E-01	-4.6986	
6	0.925	-.6719648	-1.3211	.13560	-3.6564	
7	0.950	-1.964465	-.94032	.59123	-2.3824	
8	0.975	-3.018235	-.75365	1.1880	-1.7870	
9	1.000	-5.714920	-.61815	1.8460	-1.3943	
10	1.025	-3.762311	-.51055	2.3174	-1.1129	
11	1.050	-3.458299	-.42719	2.5736	-.91503	
12	1.075	-2.925289	-.35796	2.6013	-.76660	
13	1.100	-2.355057	-.29894	2.4757	-.65231	
14	1.125	-1.923671	-.25574	2.3090	-.57938	
15	1.150	-1.611573	-.20223	2.0377	-.49051	
16	1.175	-1.372208	-.16144	1.8088	-.43133	
17	1.200	-.8094422	-.12472	1.5970	-.36213	
18	1.225	-.6127643	-.91644E-01	1.4182	-.34044	
19	1.250	-.5077229	-.65236E-01	1.3230	-.31853	
20	1.275	-.3507692	-.35866E-01	1.1309	-.27430	
21	1.300	-.2658443	-.12921E-01	1.0202	-.24766	
22	1.325	-.2106342	.60506E-02	.94700	-.22879	
23	1.350	-.1558632	.23271E-01	.86332	-.20381	
24	1.375	-.1200105	.36567E-01	.80044	-.18563	
25	1.400	-.9304547E-01	.45709E-01	.75800	-.16946	
26	1.425	-.7267034E-01	.53786E-01	.71767	-.15502	
27	1.450	-.6266449E-01	.57441E-01	.69900	-.14709	
28	1.475	-.4781447E-01	.59527E-01	.67417	-.13045	
29	1.500	-.4078167E-01	.58669E-01	.66538	-.11996	
30	1.525	-.3759805E-01	.56429E-01	.66100	-.11231	
31	1.550	-.3350724E-01	.50596E-01	.65286	-.10192	
32	1.575	-.3297448E-01	.42824E-01	.65535	-.94140E-01	
33	1.600	-.3433556E-01	.35592E-01	.66700	-.87070E-01	
34	1.625	-.3716867E-01	.26243E-01	.68354	-.80620E-01	
35	1.650	-.4255678E-01	.15882E-01	.69600	-.77030E-01	
36	1.675	-.4652005E-01	.58271E-02	.73199	-.69380E-01	
37	1.700	-.5259667E-01	-.42964E-02	.76486	-.64470E-01	
38	1.725	-.5942435E-01	-.13773E-01	.79400	-.60040E-01	
39	1.750	-.6499958E-01	-.21669E-01	.83650	-.55850E-01	
40	1.775	-.7004666E-01	-.27727E-01	.87803	-.52050E-01	
41	1.800	-.7339499E-01	-.31217E-01	.92000	-.48560E-01	
42	1.825	-.7416260E-01	-.31520E-01	.96478	-.45350E-01	
43	1.850	-.7118952E-01	-.28205E-01	.99200	-.43550E-01	
44	1.875	-.6321166E-01	-.23345E-01	1.0534	-.39660E-01	
45	1.900	-.4991281E-01	-.84409E-02	1.0950	-.37140E-01	
46	1.925	-.3205967E-01	.68131E-02	1.1278	-.35260E-01	
47	1.950	-.1008975E-01	.24049E-01	1.1745	-.32640E-01	
48	1.975	.1230172E-01	.40667E-01	1.2029	-.30640E-01	
49	2.000	.3233381E-01	.55259E-01	1.2200	-.28780E-01	
50	2.025	.4753362E-01	.65726E-01	1.2298	-.27060E-01	
51	2.050	.5593776E-01	.71494E-01	1.2320	-.26090E-01	
52	2.075	.6029073E-01	.73116E-01	1.2268	-.23970E-01	
53	2.100	.5869572E-01	.70843E-01	1.2163	-.22580E-01	
54	2.125	.5311318E-01	.65691E-01	1.2039	-.21540E-01	
55	2.150	.4527543E-01	.58726E-01	1.1719	-.20090E-01	
56	2.175	.3626902E-01	.50696E-01	1.1428	-.18960E-01	
57	2.200	.2715146E-01	.42327E-01	1.1120	-.17910E-01	
58	2.225	.1848332E-01	.34111E-01	1.0770	-.16940E-01	
59	2.250	.1059113E-01	.26409E-01	1.0560	-.16380E-01	
60	2.275	.4279755E-02	.19386E-01	1.0127	-.15160E-01	
61	2.300	-.1169853E-02	.13164E-01	.98602	-.14350E-01	
62	2.325	-.5779357E-02	.77734E-02	.96700	-.13750E-01	
63	2.350	-.1016672E-01	.32343E-02	.96700	-.13750E-01	
64	2.375	-.1388944E-01	-.53070E-03	.96700	-.13750E-01	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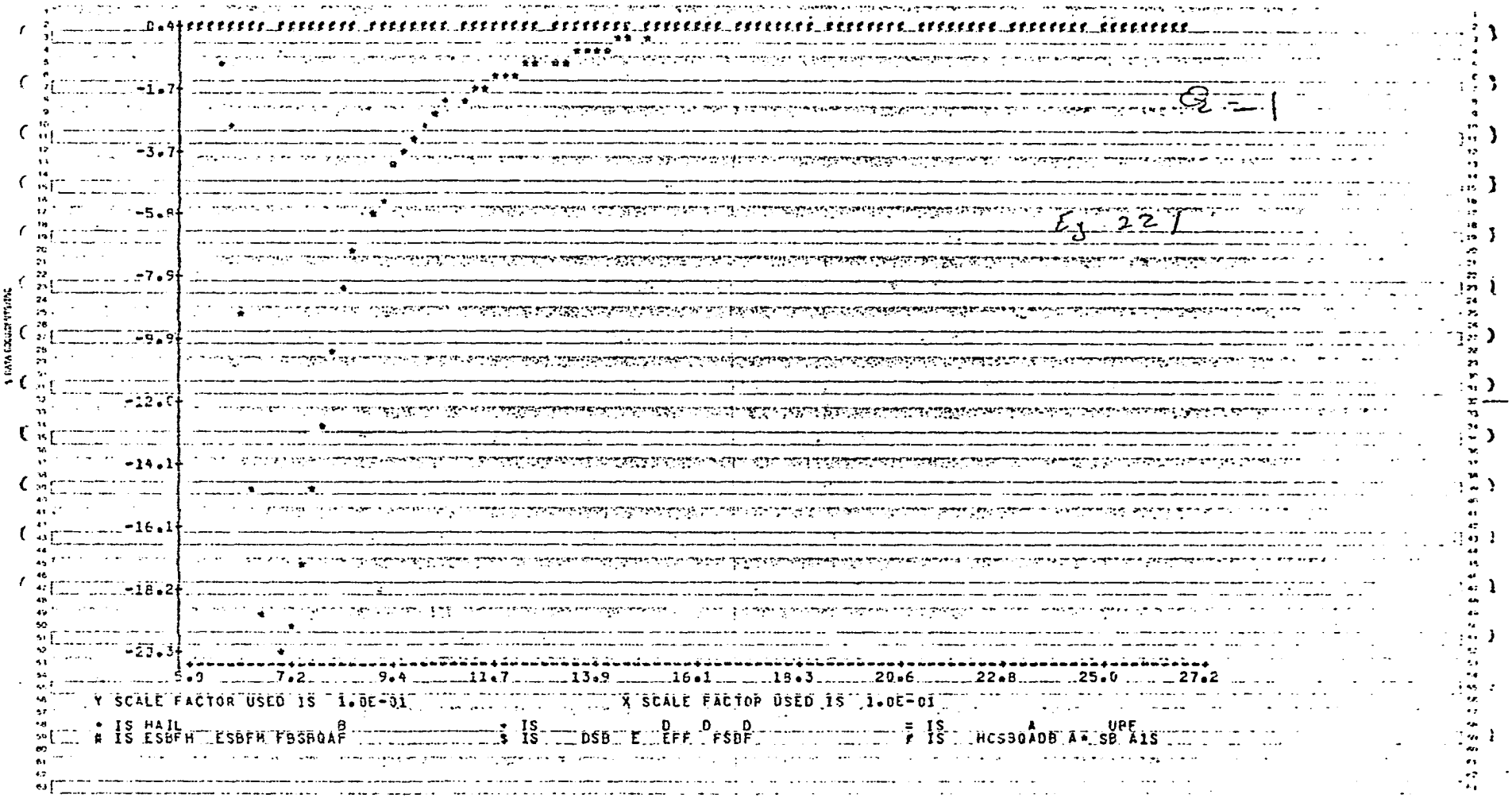
-37.6
5.0
7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Eg 22.0
Q=1
Y SCALE FACTOR USED IS 1.0E-01
X SCALE FACTOR USED IS 1.0E-01

E_g E_g $Q = 1$

1	0.800	.0	.0	.0	-31.436	
2	0.825	.0	.0	.0	-20.503	
3	0.850	.0	-.94137	.0	-9.5605	
4	0.875	.0	-.36185	.0	-4.2448	
5	0.900	-.8523923E-01	-.26245	.28250E-01	-2.7549	
6	0.925	-.3159959	-.24717	.13500	-2.0935	
7	0.950	-.9503473	-.19421	.89123	-1.4132	
8	0.975	-1.503913	-.18314	1.1880	-1.0828	
9	1.000	-1.916662	-.17909	1.8460	-.85994	
10	1.025	-2.027691	-.17740	2.3174	-.69766	
11	1.050	-1.955482	-.17894	2.5736	-.58089	
12	1.075	-1.751772	-.18158	2.6013	-.49185	
13	1.100	-1.502868	-.18484	2.4757	-.42220	
14	1.125	-1.315091	-.19243	2.3090	-.37712	
15	1.150	-1.046694	-.19212	2.0377	-.32155	
16	1.175	-.6675016	-.19555	1.8088	-.28405	
17	1.200	-.7205241	-.19961	1.5970	-.25256	
18	1.225	-.6052114	-.20109	1.4182	-.22567	
19	1.250	-.5528813	-.20646	1.3250	-.21144	
20	1.275	-.4370987	-.20393	1.1309	-.18257	
21	1.300	-.3765377	-.20402	1.0202	-.16506	
22	1.325	-.3379600	-.20416	.94700	-.15261	
23	1.350	-.2910955	-.20109	.86332	-.13608	
24	1.375	-.2555261	-.19761	.80644	-.12401	
25	1.400	-.2324012	-.19334	.75690	-.11326	
26	1.425	-.2090470	-.18756	.71787	-.10364	
27	1.450	-.1959394	-.18139	.69900	-.98350E-01	
28	1.475	-.1746073	-.17205	.67417	-.87240E-01	
29	1.500	-.1613624	-.16231	.66536	-.80230E-01	
30	1.525	-.1498477	-.15159	.66100	-.75110E-01	
31	1.550	-.1353708	-.13919	.65286	-.68160E-01	
32	1.575	-.1238621	-.12604	.65535	-.62960E-01	
33	1.600	-.1135544	-.11203	.66700	-.58220E-01	
34	1.625	-.1033677	-.97324E-01	.68354	-.53900E-01	
35	1.650	-.9316632E-01	-.82363E-01	.69600	-.51500E-01	
36	1.675	-.8275906E-01	-.66680E-01	.73199	-.46380E-01	
37	1.700	-.7209164E-01	-.51165E-01	.76486	-.43090E-01	
38	1.725	-.6077955E-01	-.35886E-01	.79400	-.40660E-01	
39	1.750	-.4881237E-01	-.20894E-01	.83856	-.37320E-01	
40	1.775	-.3636553E-01	-.66372E-02	.87003	-.34780E-01	
41	1.800	-.2370687E-01	.68795E-02	.92000	-.32450E-01	
42	1.825	-.1111744E-01	.18777E-01	.96478	-.30300E-01	
43	1.850	.2056435E-03	.29297E-01	.99200	-.29090E-01	
44	1.875	.1238307E-01	.38245E-01	1.0534	-.26490E-01	
45	1.900	.2225382E-01	.45122E-01	1.0950	-.24800E-01	
46	1.925	.2960770E-01	.49829E-01	1.1270	-.23540E-01	
47	1.950	.3604494E-01	.52490E-01	1.1745	-.21800E-01	
48	1.975	.4052766E-01	.53112E-01	1.2029	-.20460E-01	
49	2.000	.4402775E-01	.52030E-01	1.2200	-.19220E-01	
50	2.025	.4683096E-01	.49636E-01	1.2298	-.18060E-01	
51	2.050	.4856601E-01	.46274E-01	1.2320	-.17410E-01	
52	2.075	.4928812E-01	.42523E-01	1.2268	-.16090E-01	
53	2.100	.4859099E-01	.38521E-01	1.2163	-.15080E-01	
54	2.125	.4726335E-01	.34571E-01	1.2030	-.14390E-01	
55	2.150	.4549058E-01	.30895E-01	1.1719	-.13410E-01	
56	2.175	.4344497E-01	.27566E-01	1.1428	-.12650E-01	
57	2.200	.4111191E-01	.24640E-01	1.1120	-.11950E-01	
58	2.225	.3865423E-01	.22121E-01	1.0770	-.11300E-01	
59	2.250	.3614137E-02	.19971E-01	1.0560	-.10930E-01	
60	2.275	.3344654E-02	.18153E-01	1.0127	-.10110E-01	
61	2.300	.3094756E-02	.16616E-01	.98602	-.95700E-02	
62	2.325	.2848804E-02	.15322E-01	.96700	-.91700E-02	
63	2.350	.2590431E-02	.14242E-01	.96700	-.91700E-02	
64	2.375	.2401392E-02	.13321E-01	.96705	-.91700E-02	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-3.7
-5.8
-7.9
-9.9
-12.0
-14.1
-16.1
-18.2
-20.3
5.0
7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Y SCALE FACTOR USED IS 1.0E-01
X SCALE FACTOR USED IS 1.0E-01
* IS HAIL B
# IS ESBFH ESBFH FBSBQAF
$ IS DSB E EFF FSDF
= IS A UPF
F IS HCS3QADB A* SB A1S

ε_y 2 2 2 ε_y

1	0.800	.0	.0	.0	5.3403	
2	0.825	.0	.0	.0	3.9006	
3	0.850	.0	.28831E-01	.0	1.6210	
4	0.875	.0	.21100	.0	.55908	
5	0.900	.13386679E-01	.18326	.22250E-01	.29068	
6	0.925	.45106557E-01	.15367	.13500	.18089	
7	0.950	.10737765	.10918	.59123	.72440E-01	
8	0.975	.12386610	.78081E-01	1.1880	.26180E-01	
9	1.000	.94307427E-01	.52378E-01	1.8460	-.12900E-02	
10	1.025	.28321697E-01	.30941E-01	2.3174	-.18720E-01	
11	1.050	-.38667527E-01	.13739E-01	2.5736	-.28740E-01	
12	1.075	-.90438747E-01	.17551E-03	2.6013	-.34580E-01	
13	1.100	-.12176663	.11253E-01	2.4757	-.37660E-01	
14	1.125	-.13085517	.17950E-01	2.3090	-.38720E-01	
15	1.150	-.13289501	.22297E-01	2.0377	-.38920E-01	
16	1.175	-.12494566	.30906E-01	1.6088	-.36170E-01	
17	1.200	-.11311127	.33908E-01	1.5970	-.36920E-01	
18	1.225	-.10055590	.35530E-01	1.4182	-.35370E-01	
19	1.250	-.87979227E-01	.34437E-01	1.3230	-.34330E-01	
20	1.275	-.76020294E-01	.35410E-01	1.1309	-.31810E-01	
21	1.300	-.65254677E-01	.33982E-01	1.0202	-.29970E-01	
22	1.325	-.56755353E-01	.31430E-01	.94700	-.28500E-01	
23	1.350	-.47955988E-01	.29176E-01	.86332	-.26370E-01	
24	1.375	-.40897137E-01	.26043E-01	.80644	-.24670E-01	
25	1.400	-.34596636E-01	.22592E-01	.75860	-.23050E-01	
26	1.425	-.29033196E-01	.18934E-01	.71787	-.21510E-01	
27	1.450	-.24812887E-01	.14668E-01	.68909	-.20630E-01	
28	1.475	-.20276037E-01	.11369E-01	.67417	-.18700E-01	
29	1.500	-.16693011E-01	.76379E-02	.66538	-.17450E-01	
30	1.525	-.13540035E-01	.39842E-02	.66100	-.16500E-01	
31	1.550	-.10322367E-01	.64300E-03	.65286	-.15170E-01	
32	1.575	-.76391315E-02	.24999E-02	.65535	-.14150E-01	
33	1.600	-.52386624E-02	.53446E-02	.66700	-.13200E-01	
34	1.625	-.30525361E-02	.78542E-02	.68354	-.12320E-01	
35	1.650	-.12738191E-03	.99897E-02	.69600	-.11820E-01	
36	1.675	-.75665866E-03	.11784E-01	.73199	-.10750E-01	
37	1.700	-.23993191E-02	.13177E-01	.76486	-.10040E-01	
38	1.725	-.69400911E-02	.14163E-01	.79400	-.95100E-02	
39	1.750	-.10672475E-02	.14823E-01	.83653	-.87800E-02	
40	1.775	-.60158254E-02	.15099E-01	.87803	-.82200E-02	
41	1.800	-.67446877E-02	.15034E-01	.92000	-.77000E-02	
42	1.825	-.71809188E-02	.14653E-01	.96478	-.72100E-02	
43	1.850	-.69599866E-02	.13935E-01	.99200	-.69400E-02	
44	1.875	-.71299555E-02	.13110E-01	1.0534	-.63500E-02	
45	1.900	-.66264117E-02	.12042E-01	1.0956	-.58600E-02	
46	1.925	-.58249015E-02	.10839E-01	1.1270	-.56700E-02	
47	1.950	-.51503247E-02	.96620E-02	1.1745	-.52700E-02	
48	1.975	-.42671417E-02	.84974E-02	1.2029	-.49500E-02	
49	2.000	-.33709136E-02	.74271E-02	1.2200	-.46600E-02	
50	2.025	-.25677835E-02	.64780E-02	1.2298	-.43900E-02	
51	2.050	-.17737477E-02	.56022E-02	1.2320	-.42400E-02	
52	2.075	-.12816331E-02	.49547E-02	1.2268	-.39100E-02	
53	2.100	-.79545363E-03	.43340E-02	1.2163	-.36800E-02	
54	2.125	-.33955425E-03	.37673E-02	1.2039	-.35100E-02	
55	2.150	-.54310991E-05	.32720E-02	1.1719	-.32800E-02	
56	2.175	-.33415176E-03	.28077E-02	1.1424	-.31000E-02	
57	2.200	-.61019677E-03	.23813E-02	1.1126	-.29300E-02	
58	2.225	-.85966510E-03	.19818E-02	1.0770	-.27800E-02	
59	2.250	-.11514355E-02	.15996E-02	1.0569	-.26900E-02	
60	2.275	-.12625140E-02	.12433E-02	1.0127	-.24500E-02	
61	2.300	-.14423468E-02	.89923E-03	.98602	-.23500E-02	
62	2.325	-.16330128E-02	.57126E-03	.96700	-.22600E-02	
63	2.350	-.19353235E-02	.25863E-03	.96700	-.22600E-02	
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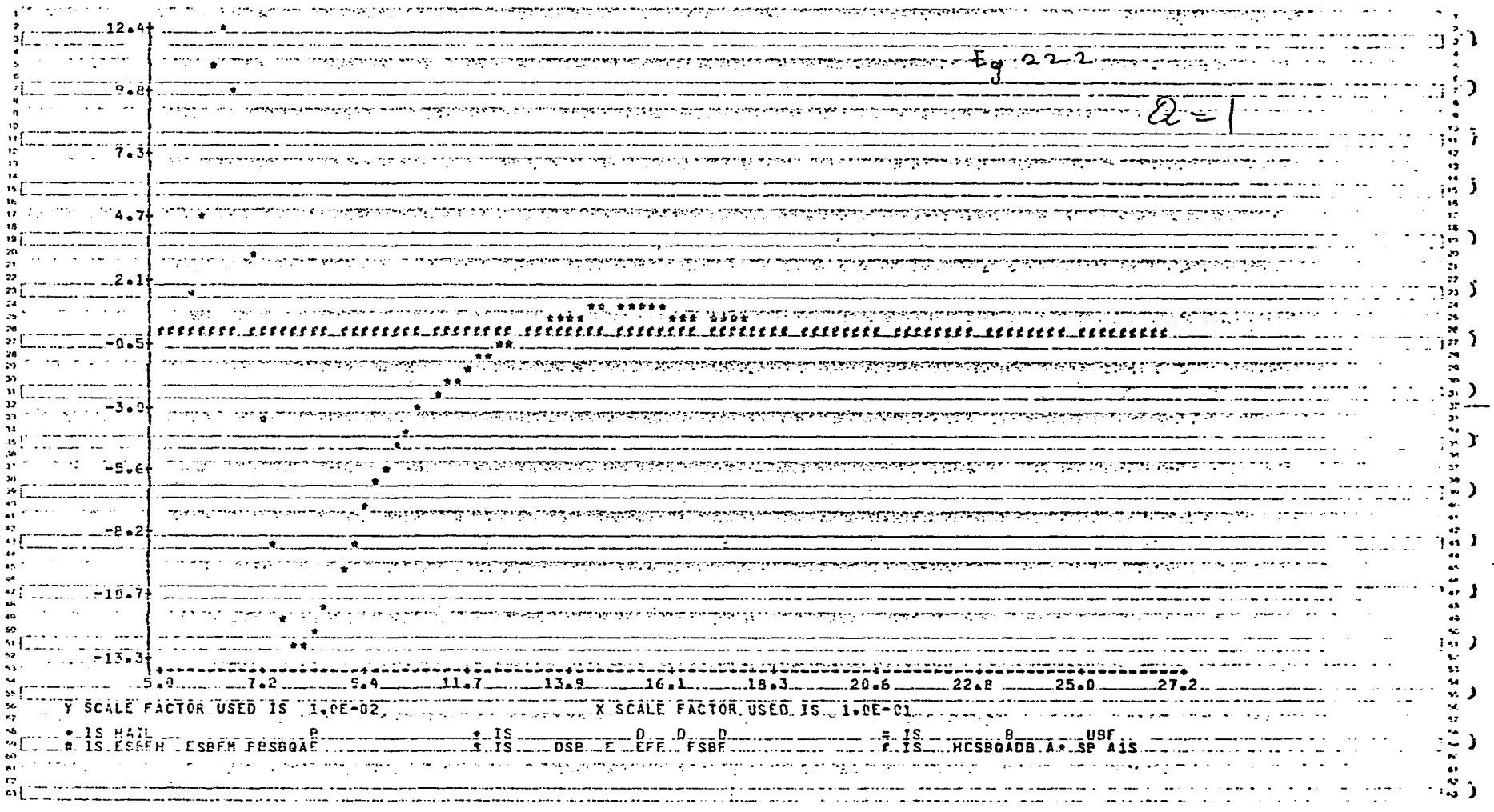
Q = 1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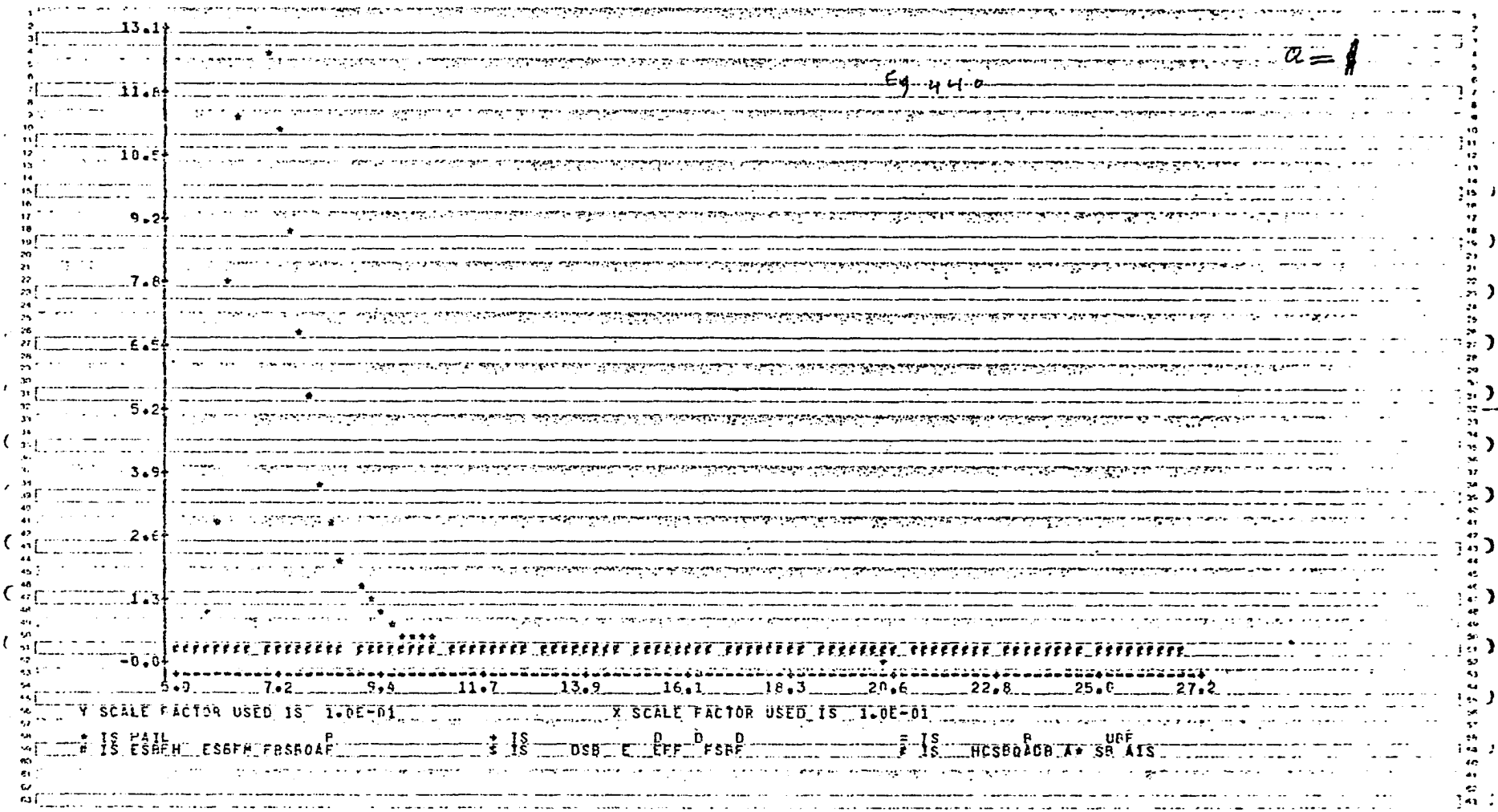
-10.7
-13.3
5.0
7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Y SCALE FACTOR USED IS 1.0E-02
X SCALE FACTOR USED IS 1.0E-01
* IS HAIL B
# IS ESBFH FSBFH FBSBQAF
* IS D D D
# IS OSB E EFF FSBF
= IS B UBF
IS HCSBQADB A* SP AIS

Eg a ≈ 1.000

T = 1.294

Ey 4	4	0			
1	0.800	.0	.0	.0	48.469
2	0.825	.0	.0	.0	30.304
3	0.850	.0	.79570E-01	.0	12.147
4	0.875	.0	.20885	.0	3.4531
5	0.900	.6064085E-01	.25017	.28250E-01	2.6044
6	0.925	.2866949	.27437	.13500	1.8489
7	0.950	.7727686	.22371	.59123	1.0833
8	0.975	1.122534	.19884	1.1880	.74607
9	1.000	1.307882	.17509	1.8460	.53341
10	1.025	1.248080	.15162	2.3174	.36694
11	1.050	1.084515	.13165	2.5735	.28975
12	1.075	.8697222	.11376	2.6013	.22061
13	1.100	.6643031	.97934E-01	2.4757	.17039
14	1.125	.5253882	.87299E-01	2.3090	.14024
15	1.150	.3623666	.72164E-01	2.0377	.10567
16	1.175	.2644911	.61008E-01	1.8088	.84410E-01
17	1.200	.1932160	.52987E-01	1.5970	.68000E-01
18	1.225	.1426419	.45502E-01	1.4162	.35080E-01
19	1.250	.1192869	.41434E-01	1.3230	.48730E-01
20	1.275	.8018154E-01	.34060E-01	1.1309	.36840E-01
21	1.300	.6131957E-01	.29765E-01	1.0202	.30340E-01
22	1.325	.5007554E-01	.26792E-01	.94700	.26080E-01
23	1.350	.3811192E-01	.23286E-01	.86332	.20960E-01
24	1.375	.3079653E-01	.20798E-01	.80649	.17390E-01
25	1.400	.2516476E-01	.18639E-01	.75000	.14560E-01
26	1.425	.2075218E-01	.16588E-01	.71787	.12220E-01
27	1.450	.1833869E-01	.15216E-01	.69900	.11020E-01
28	1.475	.1465243E-01	.13044E-01	.67417	.86300E-02
29	1.500	.1235983E-01	.11206E-01	.66538	.73700E-02
30	1.525	.1049071E-01	.94010E-02	.65100	.64700E-02
31	1.550	.8314822E-02	.74061E-02	.65286	.53300E-02
32	1.575	.6591886E-02	.55086E-02	.65535	.45500E-02
33	1.600	.5059686E-02	.36857E-02	.66700	.39000E-02
34	1.625	.3657603E-02	.20110E-02	.68354	.33900E-02
35	1.650	.2560772E-02	.62927E-03	.69600	.30500E-02
36	1.675	.1394155E-02	-.56539E-03	.73193	.24700E-02
37	1.700	.6345680E-03	-.13396E-02	.76486	.21300E-02
38	1.725	.1568095E-03	-.17025E-02	.79400	.19000E-02
39	1.750	-.1118460E-03	-.17434E-02	.83850	.16100E-02
40	1.775	-.2776113E-04	-.14316E-02	.87803	.14000E-02
41	1.800	.3084603E-03	-.87472E-03	.92000	.12100E-02
42	1.825	.8585253E-03	-.16972E-03	.96478	.10600E-02
43	1.850	.1605096E-02	.63804E-03	.99200	.98000E-03
44	1.875	.2253622E-02	.13297E-02	1.0534	.51000E-03
45	1.900	.3003665E-02	.20338E-02	1.0950	.71000E-03
46	1.925	.3754719E-02	.26916E-02	1.1270	.64000E-03
47	1.950	.4454311E-02	.32426E-02	1.1745	.55300E-03
48	1.975	.5006615E-02	.36821E-02	1.2029	.48000E-03
49	2.000	.5385566E-02	.39623E-02	1.2200	.43000E-03
50	2.025	.5959188E-02	.40591E-02	1.2298	.38000E-03
51	2.050	.5323496E-02	.39710E-02	1.2320	.35000E-03
52	2.075	.4989729E-02	.37673E-02	1.2268	.30300E-03
53	2.100	.4477035E-02	.34210E-02	1.2163	.26000E-03
54	2.125	.3877849E-02	.29835E-02	1.2030	.24000E-03
55	2.150	.3194275E-02	.25158E-02	1.1719	.21000E-03
56	2.175	.2530893E-02	.20347E-02	1.1426	.18300E-03
57	2.200	.1925368E-02	.15714E-02	1.1120	.16300E-03
58	2.225	.1370398E-02	.11298E-02	1.0770	.15000E-03
59	2.250	.8756966E-03	.68921E-03	1.0500	.14000E-03
60	2.275	.3859856E-03	.26105E-03	1.0127	.12000E-03
61	2.300	-.5366449E-04	-.16443E-03	.98602	.11000E-03
62	2.325	-.4525569E-03	-.56807E-03	.96700	.10000E-03
63	2.350	-.8021091E-03	-.92948E-03	.96700	.10000E-03
64	2.375	-.1085738E-02	-.12228E-02	.96700	.10000E-03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16.1
18.3
20.6
22.8
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Eq 44-0
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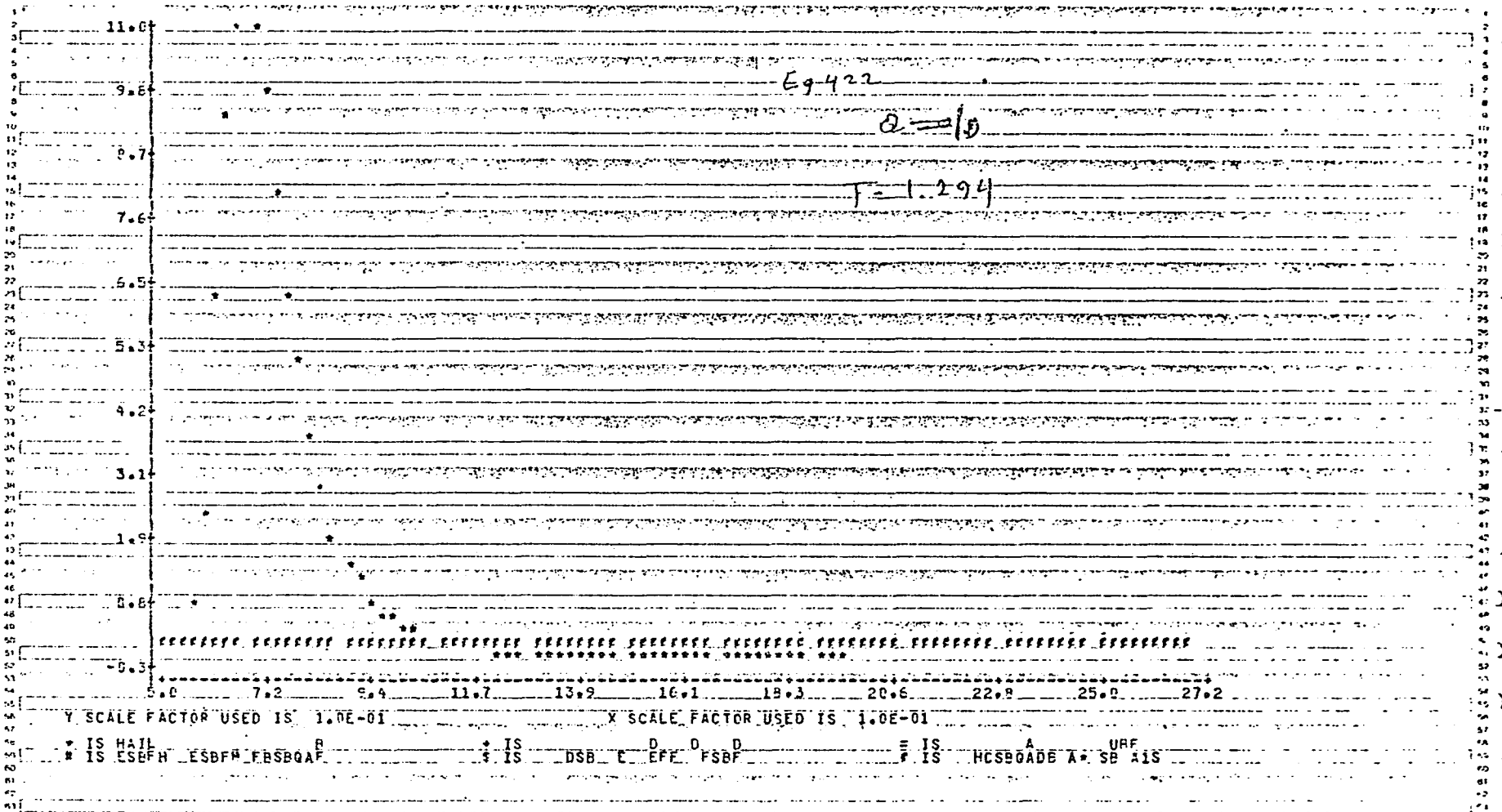
X SCALE FACTOR USED IS 1.0E-01

T=1.294
Q=1808


Eq 422
a = 15
f = 1.294
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-0.3
5.0
7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Y SCALE FACTOR USED IS 1.0E-01
X SCALE FACTOR USED IS 1.0E-01
* IS HAIL
# IS ESBFH ESBFM EBSBQAF
+ IS
$ IS DSB E EFE FSBF
= IS A URF
F IS HCSBQADE A* SB AIS

E_3 E_g $a = 0.4$

$Q = 1$

$T = 1.294$

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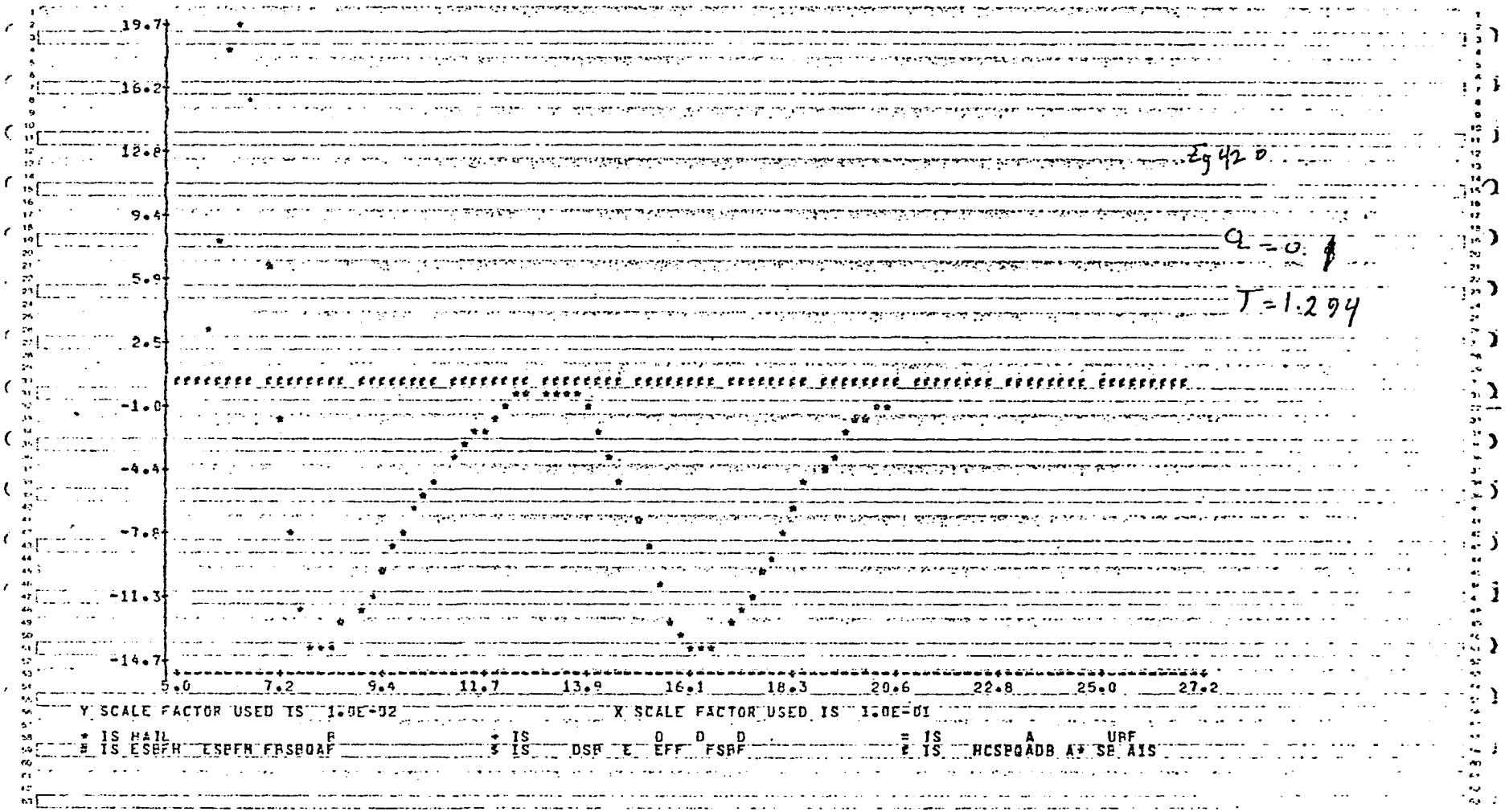
2	0.875	.0	.0	.0	-3.6875	
3	0.900	.0	6.3954	.0	-1.2633	
4	0.925	.0	2.2459	.0	-.33069	
5	0.950	.2831700E-01	1.1427	.2825OE-01	-.14036	
6	0.975	.7755148E-01	.64813	.13500	-.73670E-01	
7	0.550	.1805698	.31584	.59123	-.10130E-01	
8	0.975	.1967269	.15490	1.1880	.10700E-01	
9	1.000	.1492188	.60744E-01	1.8469	.20090E-01	
10	1.025	.6518704E-01	.34391E-02	2.3174	.24290E-01	
11	1.050	-.1693288E-01	-.21167E-01	2.5736	.24830E-01	
12	1.075	-.8244312E-01	-.55023E-01	2.6013	.23830E-01	
13	1.100	-.1212112	-.75599E-01	2.4757	.22040E-01	
14	1.125	-.1462847	-.83691E-01	2.3090	.20320E-01	
15	1.150	-.1446681	-.80707E-01	2.0377	.17700E-01	
16	1.175	-.1409165	-.93485E-01	1.8008	.15580E-01	
17	1.200	-.1323422	-.96469E-01	1.5970	.13600E-01	
18	1.225	-.1220966	-.97908E-01	1.4182	.11820E-01	
19	1.250	-.1174229	-.99594E-01	1.3230	.10840E-01	
20	1.275	-.9371197E-01	-.96699E-01	1.1309	.88360E-02	
21	1.300	-.8220777E-01	-.94140E-01	1.0202	.76000E-02	
22	1.325	-.7954049E-01	-.90732E-01	.94700	.57400E-02	
23	1.350	-.6662954E-01	-.85347E-01	.85332	.56200E-02	
24	1.375	-.6001404E-01	-.79273E-01	.80644	.48300E-02	
25	1.400	-.5166155E-01	-.72266E-01	.75000	.41500E-02	
26	1.425	-.4362946E-01	-.64347E-01	.71787	.35700E-02	
27	1.450	-.3693347E-01	-.5605SE-01	.69900	.32600E-02	
28	1.475	-.2984448E-01	-.46908E-01	.67417	.26400E-02	
29	1.500	-.2371117E-01	-.37506E-01	.66538	.22700E-02	
30	1.525	-.1778345E-01	-.29226E-01	.66109	.20200E-02	
31	1.550	-.1265148E-01	-.21140E-01	.65286	.17000E-02	
32	1.575	-.8772206E-02	-.14253E-01	.65535	.14700E-02	
33	1.600	-.5132316E-02	-.89647E-02	.66700	.12700E-02	
34	1.625	-.3153435E-02	-.57134E-02	.68354	.11050E-02	
35	1.650	-.2724592E-02	-.49246E-02	.69600	.10150E-02	
36	1.675	-.4410267E-02	-.68550E-02	.73199	.83000E-03	
37	1.700	-.8468308E-02	-.11752E-01	.76486	.73000E-03	
38	1.725	-.1520224E-01	-.19796E-01	.79400	.65000E-03	
39	1.750	-.2538666E-01	-.30757E-01	.83950	.55000E-03	
40	1.775	-.3850938E-01	-.44339E-01	.87803	.48000E-03	
41	1.800	-.5473650E-01	-.59916E-01	.92000	.42000E-03	
42	1.825	-.7346138E-01	-.76534E-01	.96478	.37000E-03	
43	1.850	-.9175599E-01	-.92635E-01	.99200	.34000E-03	
44	1.875	-.1126498	-.10723	1.0534	.29000E-03	
45	1.900	-.1290284	-.11808	1.0950	.25000E-03	
46	1.925	-.1397924	-.12427	1.1270	.23000E-03	
47	1.950	-.1471253	-.12546	1.1745	.19000E-03	
48	1.975	-.1466782	-.12227	1.2029	.17000E-03	
49	2.000	-.1413036	-.11597	1.2200	.15000E-03	
50	2.025	-.1327797	-.10810	1.2298	.13000E-03	
51	2.050	-.1230211	-.99575E-01	1.2320	.12000E-03	
52	2.075	-.1129011	-.92130E-01	1.2268	.10000E-03	
53	2.100	-.1027883	-.84612E-01	1.2163	.10000E-03	
54	2.125	-.9248149E-01	-.76966E-01	1.2030	.90000E-04	
55	2.150	-.8060223E-01	-.66852E-01	1.1719	.70000E-04	
56	2.175	-.6995566E-01	-.60411E-01	1.1428	.70000E-04	
57	2.200	-.5773336E-01	-.51951E-01	1.1120	.60000E-04	
58	2.225	-.4711491E-01	-.43796E-01	1.0770	.50000E-04	
59	2.250	-.3810243E-01	-.36208E-01	1.0560	.50000E-04	
60	2.275	-.2971240E-01	-.29360E-01	1.0127	.40000E-04	
61	2.300	-.2311648E-01	-.23484E-01	.98602	.40000E-04	
62	2.325	-.1793008E-01	-.18582E-01	.96700	.40000E-04	
63	2.350	-.1411032E-01	-.14632E-01	.96700	.40000E-04	
64	2.375	-.1118332E-01	-.11605E-01	.96700	.40000E-04	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9.4
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2.5
-1.0
-4.4
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-11.3
-14.7
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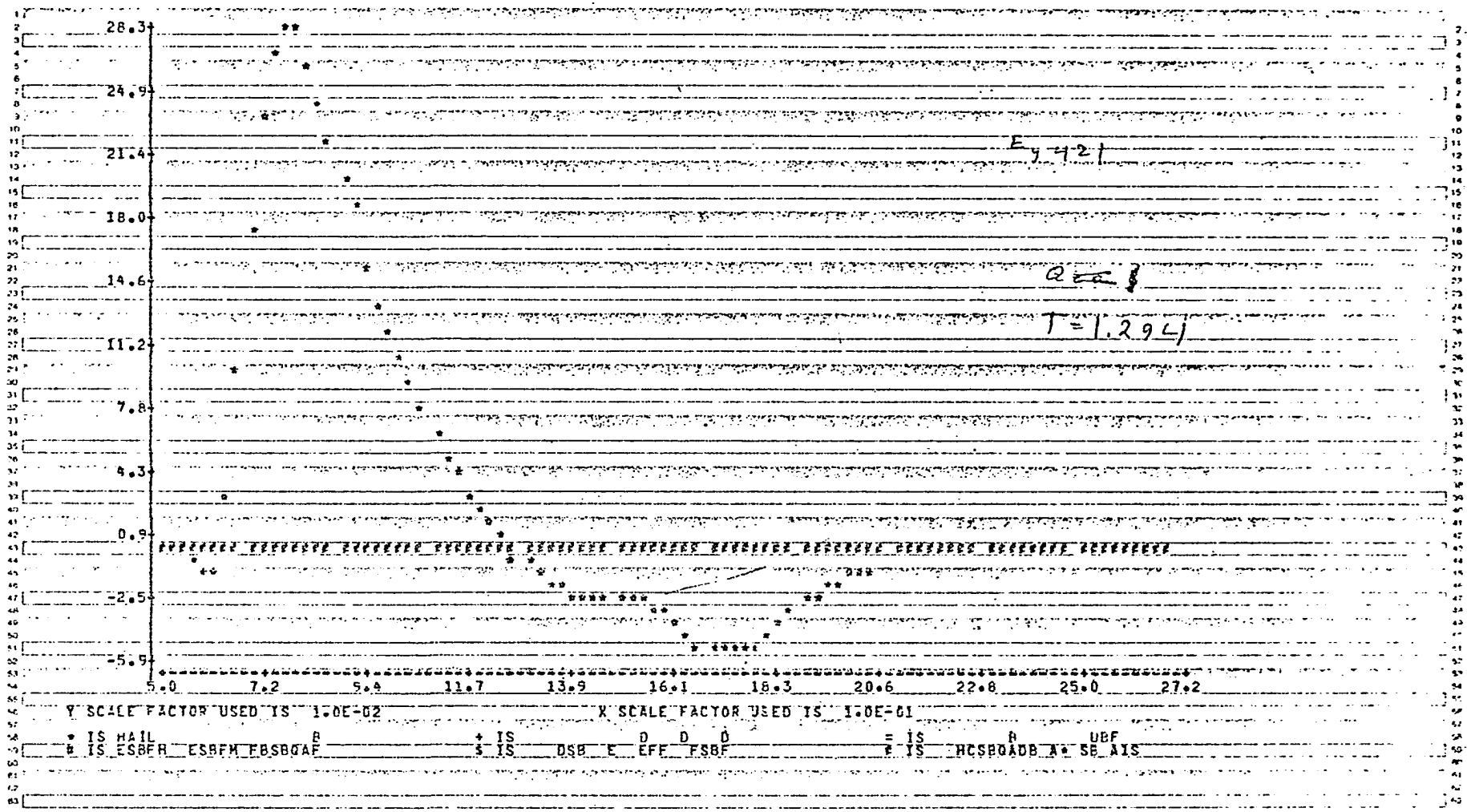
7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Eg 42 0
q = 0.
T = 1.294
Y SCALE FACTOR USED IS 1.0E-02
X SCALE FACTOR USED IS 1.0E-01
* IS HAIL
$ IS ESBFR ESBFR FBSBOAF
+ IS
$ IS DSF E EFF FSBF
D D D
= IS
£ IS HCSBQADB A* SB AIS
A
URF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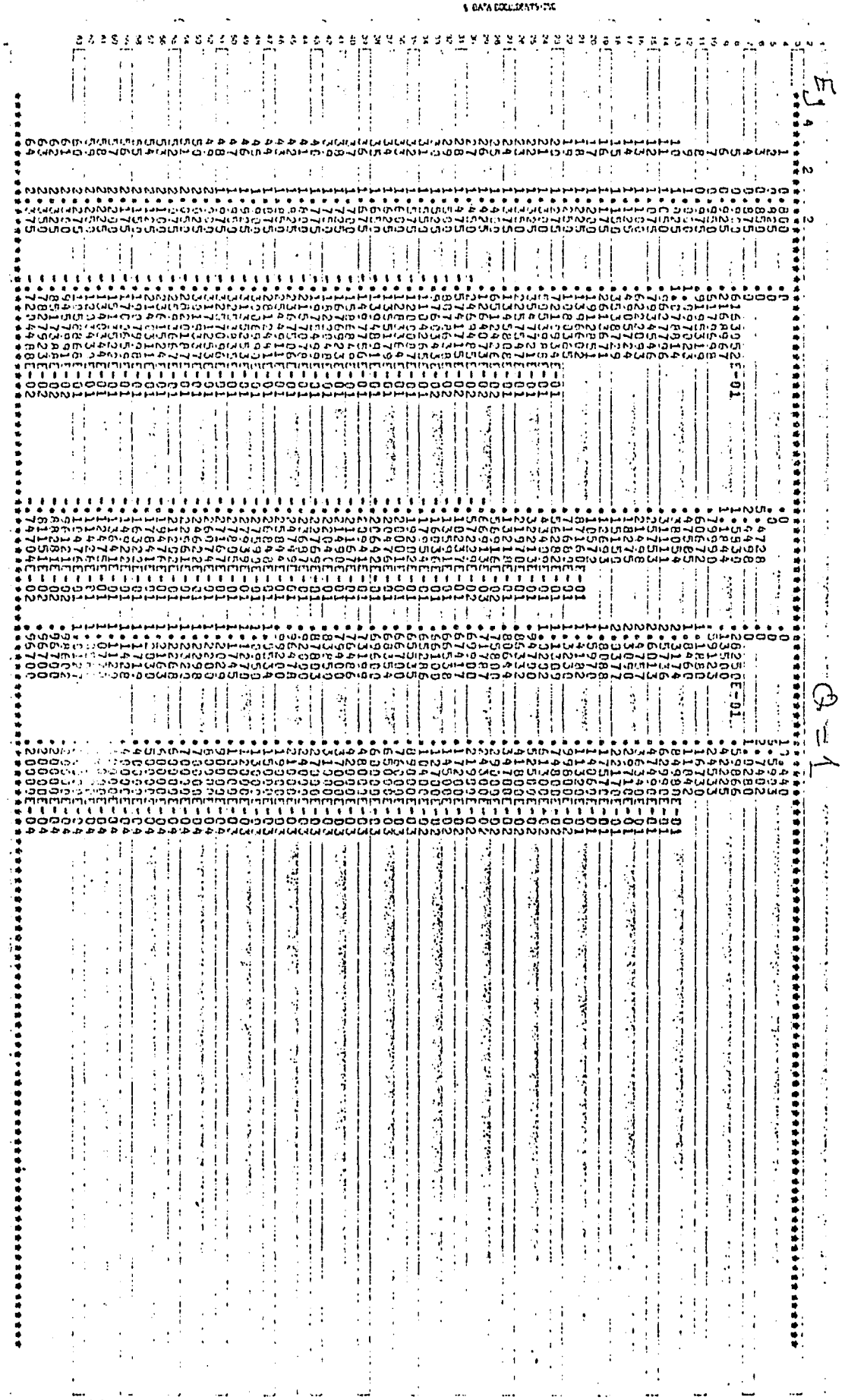
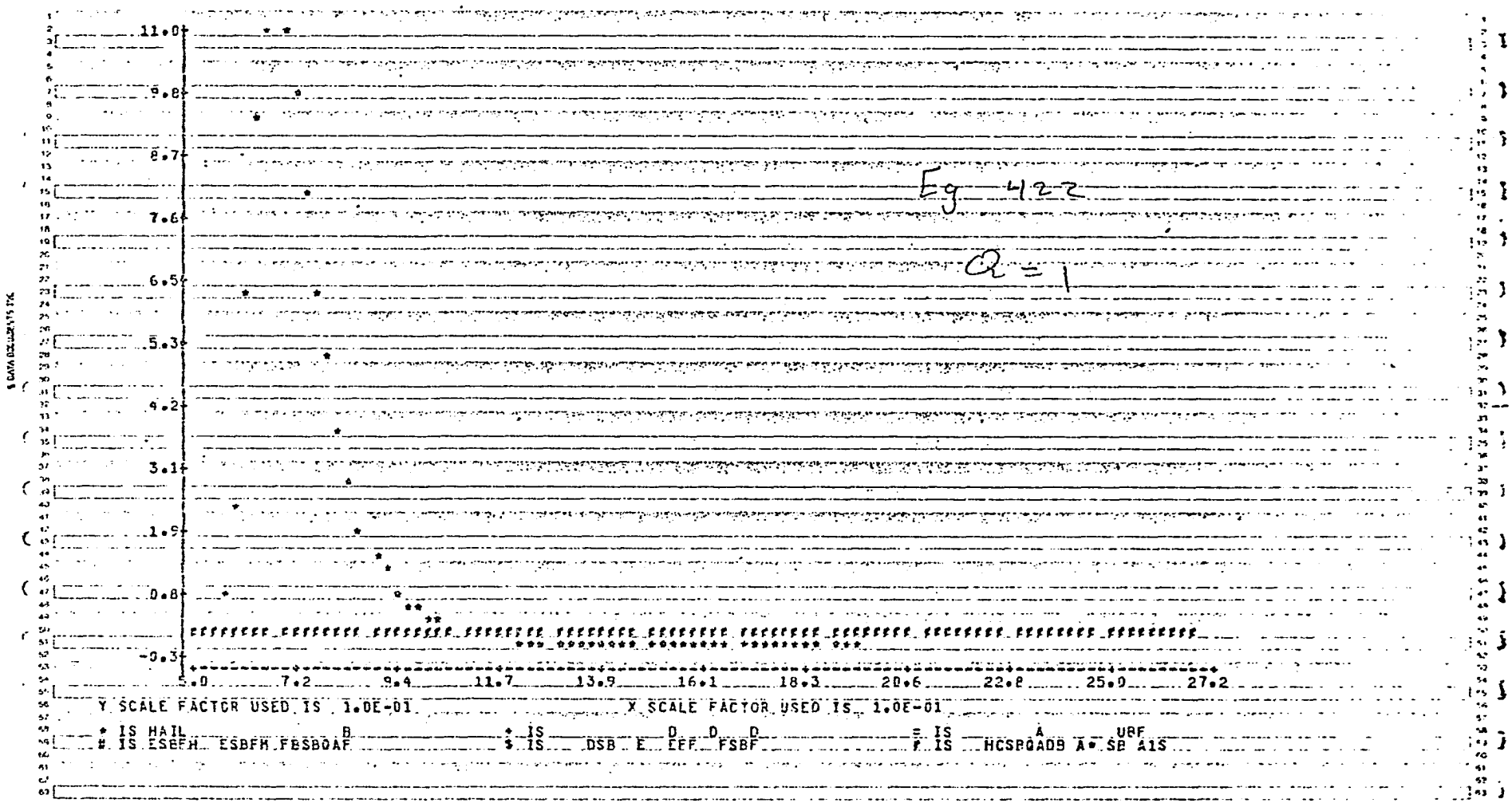
14.6
11.2
7.8
4.3
0.9
-2.5
-5.9
5.0
7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Y SCALE FACTOR USED IS 1.0E-02
X SCALE FACTOR USED IS 1.0E-01
E y 42
Q = 8
T = 1.294

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7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Eg 422
Q = 1
Y SCALE FACTOR USED IS 1.0E-01
X SCALE FACTOR USED IS 1.0E-01
* IS HAIL
# IS ESBFH ESBFH FBSBOAF
+ IS
$ IS DSB E EFF FSBF
= IS
F IS HCSBOADB A SB A1S
A
URF

Eg

4 4 0

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2	0.825	.0	.0	.0	30.304	
3	0.850	.0	.79570E-01	.0	12.147	
4	0.875	.0	.20885	.0	4.4531	
5	0.900	.80640B5E-01	.25017	.28250E-01	2.6044	
6	0.925	.2866449	.27437	.13500	1.0489	
7	0.950	.77276B6	.22371	.59123	1.0833	
8	0.975	1.1229538	.19884	1.1880	.74607	
9	1.000	1.3078882	.17509	1.8460	.53341	
10	1.025	1.2480860	.15162	2.3174	.38694	
11	1.050	1.0845515	.13165	2.5736	.28975	
12	1.075	.8697922	.11376	2.6013	.22061	
13	1.100	.6643031	.97934E-01	2.4757	.17039	
14	1.125	.5253882	.87299E-01	2.3090	.14024	
15	1.150	.3623666	.72164E-01	2.0377	.10567	
16	1.175	.2644811	.61806E-01	1.8088	.84410E-01	
17	1.200	.1932160	.52987E-01	1.5970	.68000E-01	
18	1.225	.1426419	.45502E-01	1.4182	.55060E-01	
19	1.250	.1192869	.41434E-01	1.3230	.48730E-01	
20	1.275	.8018154E-01	.34960E-01	1.1309	.36800E-01	
21	1.300	.6131957E-01	.29765E-01	1.0202	.30340E-01	
22	1.325	.5007554E-01	.25790E-01	.94700	.26080E-01	
23	1.350	.3811192E-01	.23286E-01	.86332	.20860E-01	
24	1.375	.3079653E-01	.20799E-01	.80644	.17290E-01	
25	1.400	.2516476E-01	.18639E-01	.75800	.14560E-01	
26	1.425	.2075218E-01	.16688E-01	.71787	.12220E-01	
27	1.450	.1833869E-01	.15216E-01	.69900	.11020E-01	
28	1.475	.1465243E-01	.13044E-01	.67417	.86900E-02	
29	1.500	.1235983E-01	.11206E-01	.66538	.73700E-02	
30	1.525	.1049977E-01	.94019E-02	.66100	.64700E-02	
31	1.550	.8314822E-02	.74060E-02	.65286	.53300E-02	
32	1.575	.6591086E-02	.55066E-02	.65535	.45500E-02	
33	1.600	.5059696E-02	.36857E-02	.66700	.39000E-02	
34	1.625	.3657603E-02	.20110E-02	.66154	.33400E-02	
35	1.650	.2560772E-02	.62927E-03	.69600	.30500E-02	
36	1.675	.1394155E-02	-.56539E-03	.73199	.24700E-02	
37	1.700	.6045660E-03	-.13396E-02	.76486	.21300E-02	
38	1.725	.1568045E-03	-.17025E-02	.79400	.19000E-02	
39	1.750	-.1118486E-03	-.17434E-02	.83850	.16100E-02	
40	1.775	-.2776110E-04	-.14316E-02	.87803	.14000E-02	
41	1.800	.3084603E-03	-.87472E-03	.92000	.12100E-02	
42	1.825	.8589253E-03	-.16972E-03	.96478	.10600E-02	
43	1.850	.1605096E-02	.63804E-03	.99200	.98000E-03	
44	1.875	.2253622E-02	.13293E-02	1.0834	.81000E-03	
45	1.900	.3003665E-02	.20330E-02	1.0950	.71000E-03	
46	1.925	.3754719E-02	.26916E-02	1.1270	.64000E-03	
47	1.950	.4456311E-02	.32426E-02	1.1745	.55000E-03	
48	1.975	.5006615E-02	.36021E-02	1.2029	.48000E-03	
49	2.000	.5356966E-02	.39023E-02	1.2200	.43000E-03	
50	2.025	.5459148E-02	.40591E-02	1.2258	.38000E-03	
51	2.050	.5323495E-02	.39710E-02	1.2320	.35000E-03	
52	2.075	.4989728E-02	.37673E-02	1.2268	.30000E-03	
53	2.100	.4477035E-02	.34210E-02	1.2163	.26000E-03	
54	2.125	.3877845E-02	.29835E-02	1.2030	.24000E-03	
55	2.150	.3194275E-02	.25158E-02	1.1719	.21000E-03	
56	2.175	.2530893E-02	.20347E-02	1.1428	.18000E-03	
57	2.200	.1925568E-02	.15714E-02	1.1120	.16000E-03	
58	2.225	.1378839E-02	.11298E-02	1.0770	.15000E-03	
59	2.250	.8756486E-03	.68921E-03	1.0560	.14000E-03	
60	2.275	.3858866E-03	.26105E-03	1.0127	.12000E-03	
61	2.300	-.5366449E-04	-.16443E-03	.98602	.11000E-03	

Q=1

Eq Q=1

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3	0.850	.0	1.4760	.0	8.5693	
4	0.875	.0	.62005	.0	3.2777	
5	0.900	.6632710E-01	.40149	.2825?E-01	1.9464	
6	0.925	.2303231	.31427	.13590	1.3918	
7	0.950	.6165810	.21240	.59123	.83048	
8	0.975	.8841906	.16640	1.1880	.57787	
9	1.000	1.018980	.13525	1.8469	.41674	
10	1.025	.9653639	.11169	2.3174	.30459	
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12	1.075	.6679822	.80854E-01	2.6013	.17592	
13	1.100	.5105565	.69724E-01	2.4757	.13656	
14	1.125	.4044440	.62480E-01	2.3098	.11268	
15	1.150	.2808039	.52566E-01	2.0377	.85240E-01	
16	1.175	.2056963	.45676E-01	1.8068	.68270E-01	
17	1.200	.1512394	.39502E-01	1.5670	.55110E-01	
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19	1.250	.9291238E-01	.30629E-01	1.3230	.39600E-01	
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21	1.300	.4661243E-01	.20970E-01	1.0202	.24720E-01	
22	1.325	.3698208E-01	.17792E-01	.94760	.21260E-01	
23	1.350	.2700942E-01	.14266E-01	.86332	.17020E-01	
24	1.375	.2071797E-01	.11491E-01	.80644	.14200E-01	
25	1.400	.1591633E-01	.91078E-02	.75900	.11890E-01	
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38	1.725	.6311309E-02	.63808E-02	.79499	.15500E-02	
39	1.750	.6462160E-02	.63966E-02	.83856	.13110E-02	
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41	1.800	.6256986E-02	.58111E-02	.92000	.99000E-03	
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43	1.850	.5372260E-02	.46157E-02	.99209	.80000E-03	
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46	1.925	.3322975E-02	.23455E-02	1.1270	.52000E-03	
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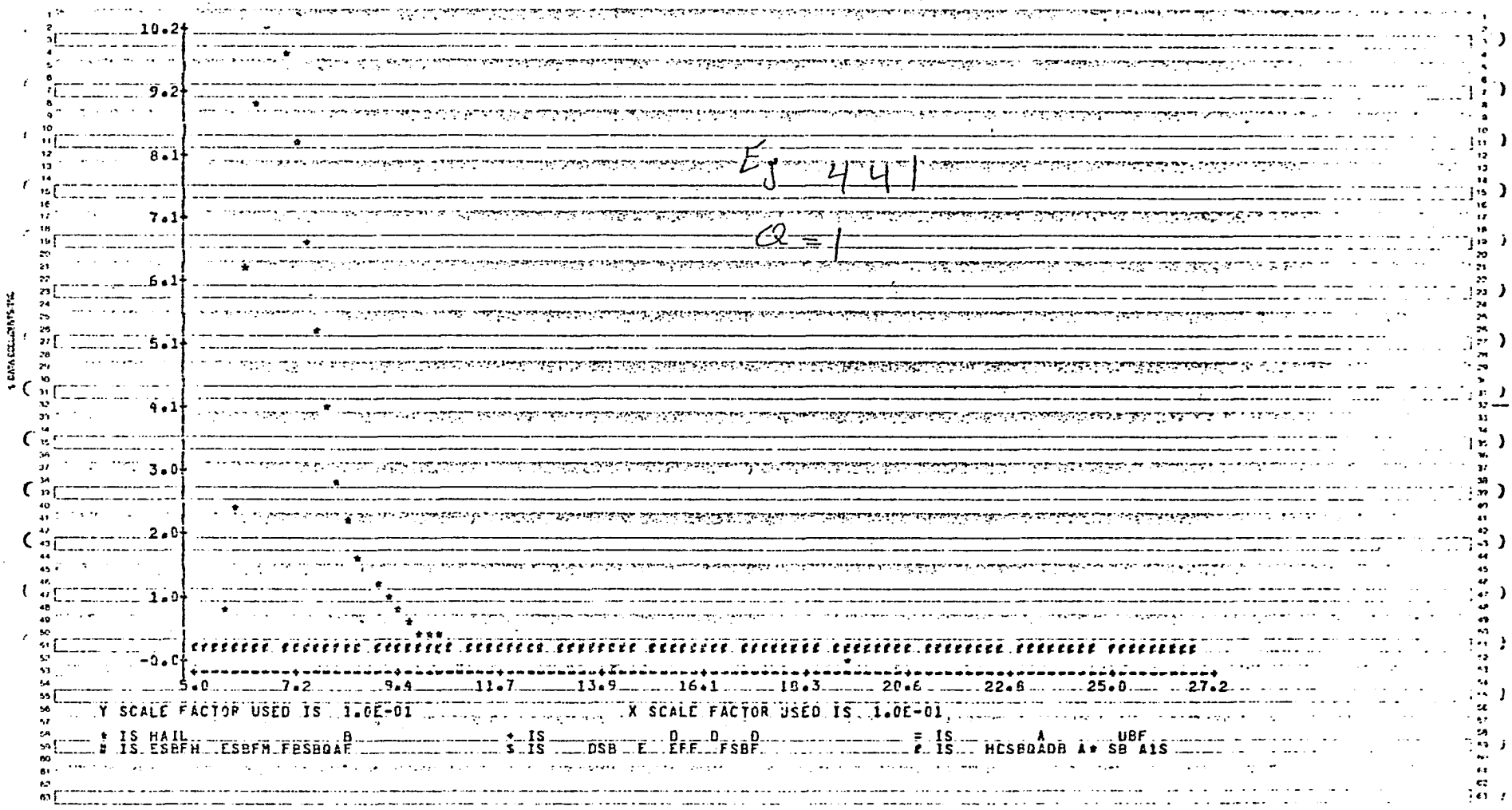
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9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
EJ 441
Q = 1
Y SCALE FACTOR USED IS 1.0E-01
X SCALE FACTOR USED IS 1.0E-01

Eg. 4 Q = 1

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3	0.850	.0	6.3954	.0	-1.2633	
4	0.875	.0	2.2450	.0	-.33069	
5	0.900	.2831700E-01	1.1427	.2825QE-01	-.14036	
6	0.925	.7755148E-01	.64813	.13500	-.73670E-01	
7	0.950	.1805698	.31554	.59123	-.10130E-01	
8	0.975	.1967260	.15490	1.1080	.10700E-01	
9	1.000	.1492189	.69744E-01	1.8480	.20050E-01	
10	1.025	.6518704E-01	.38391E-02	2.3174	.24290E-01	
11	1.050	-.1893288E-01	-.321A7E-01	2.5736	.24A30E-01	
12	1.075	-.8244312E-01	-.55523E-01	2.6013	.23830E-01	
13	1.100	-.1212112	-.70999E-01	2.4757	.22040E-01	
14	1.125	-.1463247	-.83691E-01	2.3090	.20320E-01	
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16	1.175	-.1409165	-.93485E-01	1.8088	.15580E-01	
17	1.200	-.1323422	-.96469E-01	1.5970	.13600E-01	
18	1.225	-.1220866	-.97908E-01	1.4182	.11820E-01	
19	1.250	-.1174220	-.98594E-01	1.3230	.10840E-01	
20	1.275	-.9937197E-01	-.96699E-01	1.1309	.88300E-02	
21	1.300	-.8626777E-01	-.94140E-01	1.0202	.76000E-02	
22	1.325	-.7954845E-01	-.90732E-01	.94706	.67400E-02	
23	1.350	-.6888954E-01	-.85397E-01	.86332	.56200E-02	
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25	1.400	-.5160155E-01	-.72228E-01	.75800	.41500E-02	
26	1.425	-.4362886E-01	-.64345E-01	.71787	.35700E-02	
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28	1.475	-.2984448E-01	-.46908E-01	.67417	.26400E-02	
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30	1.525	-.1796345E-01	-.29226E-01	.66100	.20200E-02	
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32	1.575	-.8377206E-02	-.14253E-01	.65535	.14700E-02	
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38	1.725	-.1520224E-01	-.19796E-01	.79400	.65000E-03	
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41	1.800	-.5473690E-01	-.59916E-01	.92000	.42000E-03	
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43	1.850	-.9175509E-01	-.92835E-01	.99200	.34000E-03	
44	1.875	-.1126498	-.10723	1.0534	.29000E-03	
45	1.900	-.1290244	-.11808	1.0850	.25000E-03	
46	1.925	-.1397924	-.12427	1.1270	.23000E-03	
47	1.950	-.1471253	-.12546	1.1745	.19000E-03	
48	1.975	-.1460782	-.12227	1.2029	.17000E-03	
49	2.000	-.1413036	-.11587	1.2200	.15000E-03	
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53	2.100	-.1027803	-.84614E-01	1.2163	.10000E-03	
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55	2.150	-.8069223E-01	-.68852E-01	1.1719	.70000E-04	
56	2.175	-.6985566E-01	-.60411E-01	1.1428	.70000E-04	
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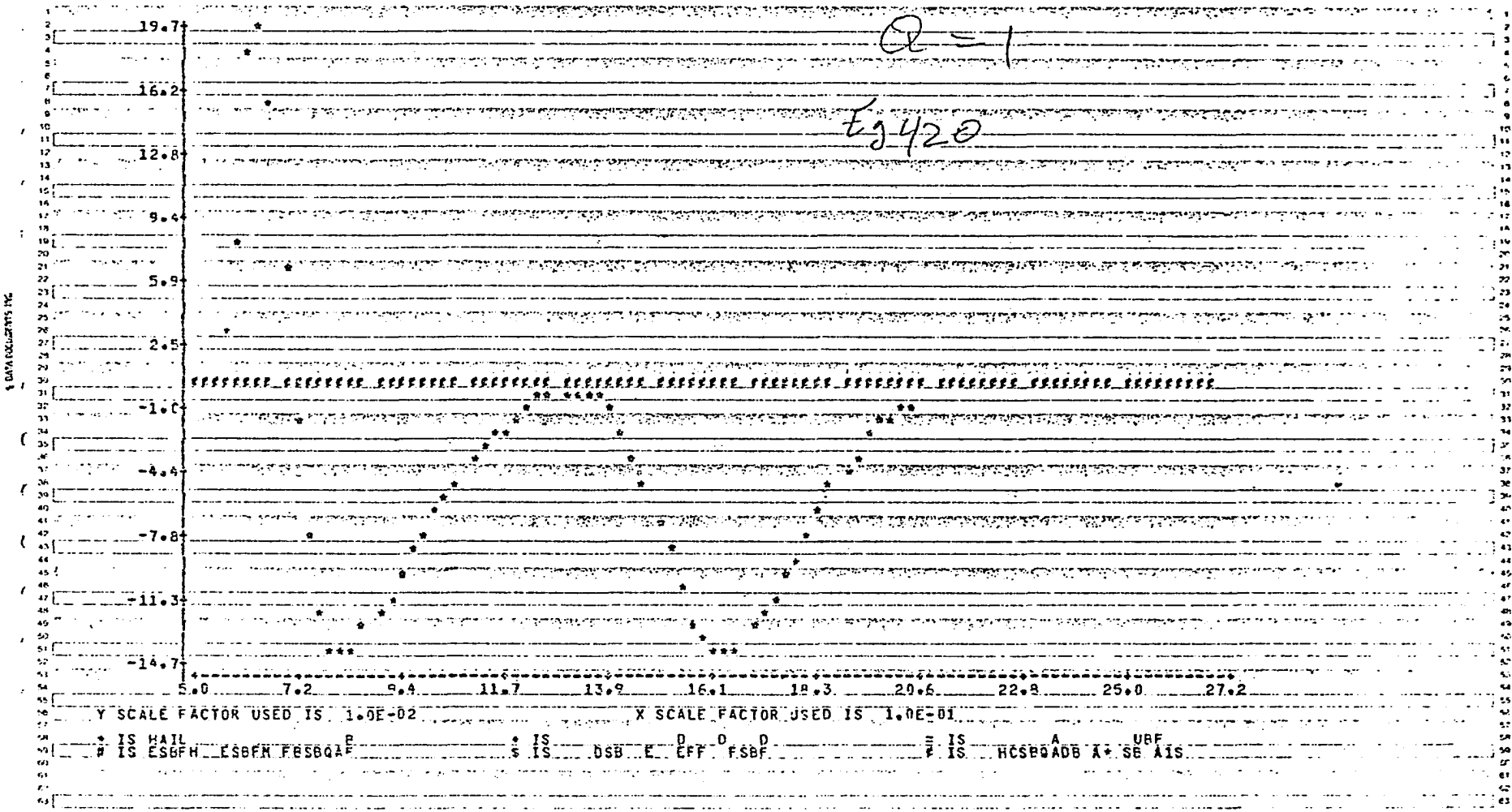
58	2.225	-.4711491E-01	-.43736E-01	1.0770	.50000E-04	
59	2.250	-.3811243E-01	-.36206E-01	1.0560	.50000E-04	
60	2.275	-.2971240E-01	-.29534E-01	1.0127	.40000E-04	
61	2.300	-.2311646E-01	-.23484E-01	.98602	.40000E-04	
62	2.325	-.1793008E-01	-.18582E-01	.96700	.40000E-04	
63	2.350	-.1411032E-01	-.14632E-01	.96700	.40000E-04	
64	2.375	-.1118332E-01	-.11605E-01	.96700	.40000E-04	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Eg 420
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12.8
9.4
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2.5
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-4.4
-7.8
-11.3
-14.7
5.0
7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Y SCALE FACTOR USED IS 1.0E-02
X SCALE FACTOR USED IS 1.0E-01
* IS HAIL
# IS ESBFH ESBFN FBSBQAF B
$ IS DSB E EFF FSBF D D D
= IS HCSBQADB A+ SB AIS UBF

Eg 4 2 1 Q = 1

1	0.800	.0	.0	.0	-.26596
2	0.825	.0	.0	.0	-.76250E-01
3	0.850	.0	-1.9583	.0	.11349
4	0.875	.0	-.70701	.0	.12668
5	0.900	-.7581074E-02	-.37513	.28250E-01	.10677
6	0.925	-.1778971E-01	-.22323	.13500	.91490E-01
7	0.950	-.1695723E-01	-.10230	.59123	.73620E-01
8	0.975	.2512251E-01	-.40073E-01	1.1880	.61220E-01
9	1.000	.9723961E-01	.16059E-02	1.8470	.51070E-01
10	1.025	.1728294	.31878E-01	2.3174	.42700E-01
11	1.050	.2331997	.54833E-01	2.5736	.35780E-01
12	1.075	.2683705	.73139E-01	2.6013	.30030E-01
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14	1.125	.2828079	.10052	2.3090	.21960E-01
15	1.150	.2695439	.11201	2.0377	.17850E-01
16	1.175	.2392070	.11759	1.8008	.15090E-01
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18	1.225	.1942279	.12627	1.4182	.10690E-01
19	1.250	.1814703	.12751	1.3230	.96600E-02
20	1.275	.1515642	.12639	1.1309	.76300E-02
21	1.300	.1323069	.12324	1.0202	.64500E-02
22	1.325	.1171059	.11801	.94700	.56500E-02
23	1.350	.9966439E-01	.11081	.86732	.46300E-02
24	1.375	.8529401E-01	.10183	.80644	.39490E-02
25	1.400	.7172605E-01	.91276E-01	.75800	.33500E-02
26	1.425	.5908225E-01	.79452E-01	.71707	.28500E-02
27	1.450	.4945827E-01	.66735E-01	.69900	.25900E-02
28	1.475	.3744388E-01	.53461E-01	.67417	.20800E-02
29	1.500	.2783398E-01	.40042E-01	.66538	.17900E-02
30	1.525	.1880011E-01	.26262E-01	.66100	.15800E-02
31	1.550	.1016691E-01	.14253E-01	.65266	.13200E-02
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36	1.675	-.2090447E-01	-.29188E-01	.73199	.63000E-03
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38	1.725	-.2704711E-01	-.34554E-01	.79400	.49000E-03
39	1.750	-.2894409E-01	-.34929E-01	.83650	.41000E-03
40	1.775	-.2968175E-01	-.34165E-01	.87803	.36000E-03
41	1.800	-.2955342E-01	-.32759E-01	.92000	.31000E-03
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43	1.850	-.2989952E-01	-.30300E-01	.99200	.25000E-03
44	1.875	-.3168762E-01	-.30290E-01	1.0534	.21000E-03
45	1.900	-.3430012E-01	-.31513E-01	1.0950	.19300E-03
46	1.925	-.3804122E-01	-.33924E-01	1.1270	.17300E-03
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49	2.000	-.5347381E-01	-.43941E-01	1.2200	.11000E-03
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51	2.050	-.5910028E-01	-.48110E-01	1.2320	.90000E-04
52	2.075	-.5911588E-01	-.48268E-01	1.2268	.80000E-04
53	2.100	-.5702357E-01	-.46954E-01	1.2163	.70000E-04
54	2.125	-.5322410E-01	-.44303E-01	1.2030	.60000E-04
55	2.150	-.4763899E-01	-.40732E-01	1.1719	.50000E-04
56	2.175	-.4184970E-01	-.36672E-01	1.1428	.50000E-04
57	2.200	-.3624182E-01	-.32632E-01	1.1120	.40000E-04
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59	2.250	-.2691850E-01	-.25531E-01	1.0560	.40000E-04
60	2.275	-.2295765E-01	-.22700E-01	1.0127	.30000E-04
61	2.300	-.2013338E-01	-.20415E-01	.98602	.30000E-04
62	2.325	-.1799241E-01	-.18636E-01	.96700	.30000E-04
63	2.350	-.1670622E-01	-.17306E-01	.96700	.30000E-04
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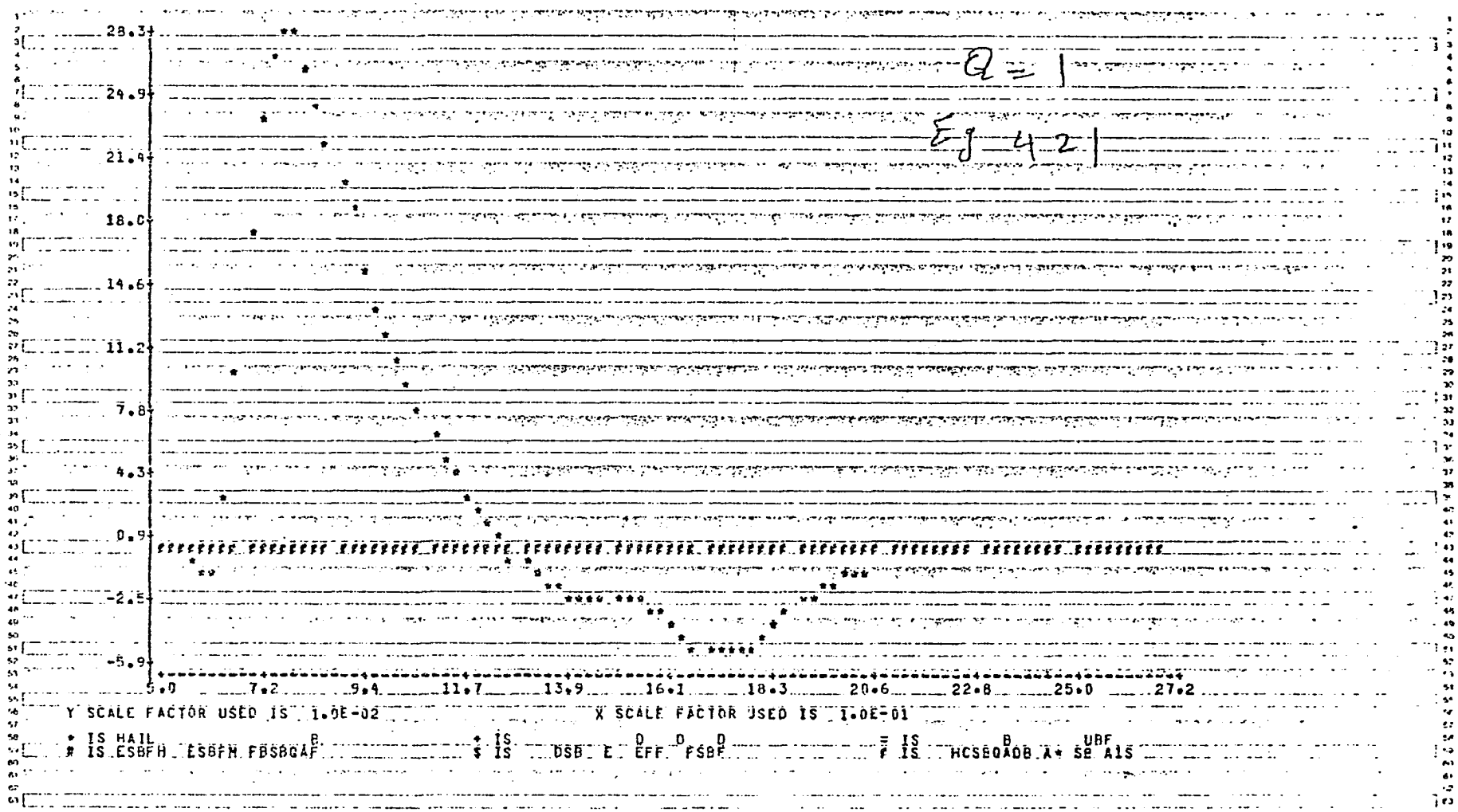
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14.6
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4.3
0.9
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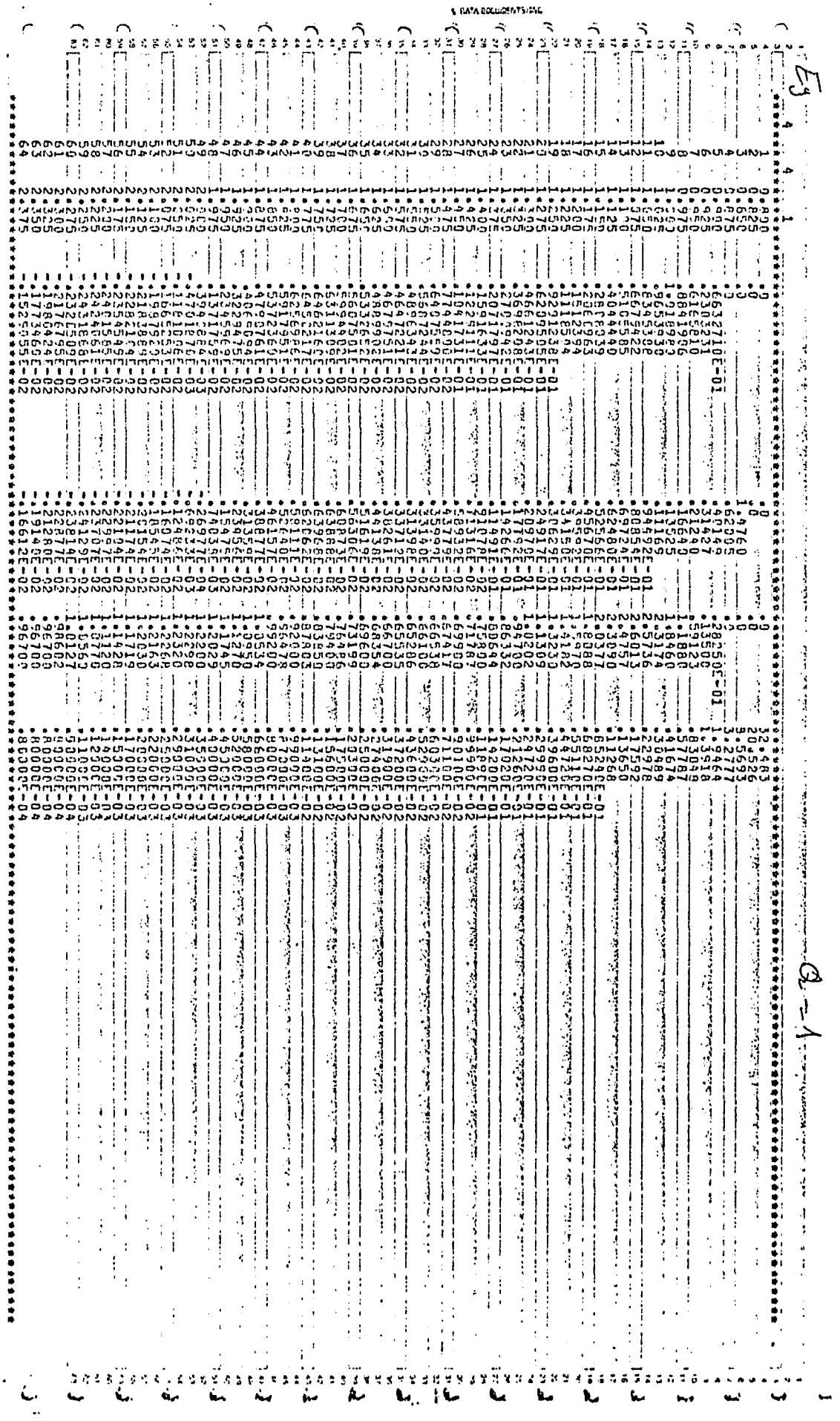
5.0
7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Y SCALE FACTOR USED IS 1.0E-02
X SCALE FACTOR USED IS 1.0E-01
* IS HAIL B
# IS ESBFH ESBFM FBSBQAF
$ IS DSB E EFF FSBF
= IS B UBF
F IS HCSBQADB A+ SE A1S



Eg 44
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8.1
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3.0
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-0.0
.0
7.2
9.4
11.7
13.9
16.1
18.3
20.6
22.8
25.0
27.2
Y SCALE FACTOR USED IS 1.0E-01
X SCALE FACTOR USED IS 1.0E-01

CONCLUSION

In this research we were looking at the first order perturbation. We looked at two cases of liquid states, one at weak quadrupole moment and the other at high. For low Q we got reasonable results. For high Q the first order perturbation appears to be inadequate.

We looked at Eg 220 and Eg 222 compared with simulation. The comparison in each case was fairly good, Eg 221 did not come as close; our results show more magnification than the simulation does.

Our theory can predict the SPH coefficients, at least qualitatively. The Lennard-Jones reference was found to be good for a low Q ($Q \leq .5$) polar fluid, for high quadrupole fluid we need to use the second order theory or other references.

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