

NUMERICAL EVALUATION OF BARRIER PENETRATION AND
RESONANCE EFFECTS ON PHASE SHIFTS ∇

by

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ABSTRACT

Quantum mechanical calculations, based on the Lennard-Jones (12,6) potential, are presented showing the dependence of the reduced phase shift, η^* , on the quantum parameter, Λ^* , for a fixed reduced effective potential and various reduced energies, E^* . The observed oscillatory behavior of $\eta^*(\Lambda^*)$ is due primarily to the inclusion of the physically unimportant contribution of $M\pi$ to the phase shift, where M is the number of quasi-bound (virtual) states of energy less than E^* . A modified reduced phase shift, $\tilde{\eta}^*$, defined by excluding this contribution, displays only the sharp inflections associated with barrier penetration under resonance conditions. Except for the resonance contribution, the phase shifts may be accurately reproduced by a second-order JWKB procedure. This method also accurately predicts the resonant energies (i.e. the energies of the quasi-bound states). The first-order JWKB treatment of the barrier penetration problem by Ford, Hill, Wakano, and Wheeler suffices for the purpose of estimating the level widths and lifetimes of the virtual states as well as the main features of the resonant phase shifts, but does not accurately reproduce the quantal calculations.

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Introduction

In the present paper, we present the results of a numerical study of phase shifts which arise in collisions between molecules which interact according to a Lennard-Jones (12,6) potential. We consider, in particular, the behavior of the phase shifts under conditions such that three classical turning points exist. Although the quantitative results apply to the present model potential, most of the qualitative features are characteristic of any realistic intermolecular potential.

The L.-J. (12,6) potential function¹ may be written

$$\varphi(r) = \epsilon \varphi^*(r/\sigma) \quad (1)$$

where

$$\varphi^*(r^*) = 4 [r^{*-12} - r^{*-6}] \quad (2)$$

ϵ is the depth of the potential minimum, σ is the separation at which the potential is zero, and $r^* = r/\sigma$ is the reduced separation. The phase shifts, η_l , are defined by the asymptotic form of the solution of the radial wave equation

$$\left\{ \frac{d^2}{dr^{*2}} + \frac{4\pi^2}{\lambda^{*2}} [E^* - \varphi^*(r^*)] - \frac{l(l+1)}{r^{*2}} \right\} r^* R_l(r^*) = 0 \quad (3)$$

in which l is the angular momentum quantum number, $R_l(r^*)$ is the radial wave function, $E^* = E/\epsilon$ is the reduced collision energy, and

$$\Lambda^* = h / [\sigma \cdot (2\mu\epsilon)^{1/2}] \quad (4)$$

is the de Boer quantum parameter.

With such a two constant potential function, the phase shifts are functions of three parameters, for example, l , E^* , and Λ^* . In the present discussion, however, it is convenient to consider a somewhat different parameterization. For this purpose, we introduce the reduced impact parameter

$$b^* = (l + \frac{1}{2}) / A = (l + \frac{1}{2}) \Lambda^* / 2\pi E^{*1/2} \quad (5)$$

where

$$A = h\sigma = 2\pi E^{*1/2} / \Lambda^* \quad (6)$$

and the reduced angular momentum

$$L^* = b^* E^{*1/2} = (l + \frac{1}{2}) \Lambda^* / 2\pi \quad (7)$$

The reduced effective potential is

$$\phi^*(r^*, L^*) = \varphi^*(r^*) + L^{*2}/r^{*2} \quad , \quad (8)$$

the sum of the true potential and the centrifugal potential, determined by L^* . We shall consider the phase shifts as functions of L^* , E^* , and Λ^* (or occasionally, ℓ).

The effective potential depends parametrically on the angular momentum, L^* . For

$$0 < L^* < 6 \cdot 5^{-5/6} = 1.5692 \quad (9)$$

this function has both a minimum and a maximum, and thus for a range of energy, three classical turning points exist. The effective potential for $L^* = (1.6)^{1/2} = 1.2649$ is illustrated in Fig. 1. For this value of the reduced angular momentum, three classical turning points exist for energies in the range

$$0.216247 < E^* < 0.400804 \quad (10)$$

All of the numerical values of the phase shifts presented in this paper refer to this value of L^* . For the most part, the calculations are restricted to nine values of the reduced energy. Five of these values are in the range leading to three classical

turning points. In addition to these values, one lower value and three higher values of the energy are considered. For the given L^* and these values of E^* , the phase shift is then considered as a function of the quantum parameter, Λ^* . Although in the figures Λ^* is considered as a continuous variable, the calculations were, of course, restricted to values of Λ^* corresponding to integer l . (The definition of the phase shift, however, may easily be generalized to non-integer values of l .)

Numerical Procedures

The phase shifts were computed by direct numerical integration^{2/} of the radial wave equation, (Eq. 3), using Runge-Kutta-Gill and de Vogelaere methods. The procedure of Ref. 2 was used except that, after four "apparent phase shifts" agreed to within 10^{-4} radian, a small "truncation" correction was added. The correction term is based on the use of a JWKB approximation to the remaining portion of wave function. The added term on the phase shift is $2A/5E^*r_N^{*5}$ where r_N^* is the value of r^* at which the numerical integration is terminated. The resulting phase shifts are believed to be accurate to ± 0.0001 radian.

Results

Table A1, of the Appendix, presents the results of these computations and a number of related quantities (to be discussed). In the classical limit ($\hbar \rightarrow 0$ or the reduced mass $\mu \rightarrow \infty$) the

quantum parameter $\Lambda^* \rightarrow 0$; the magnitude of Λ^* may, thus, be regarded as a measure of the quantum character of the collision. In the classical limit, the phase shift becomes infinite but the product $\Lambda^* \eta$ becomes of function of two parameters, which may be taken to be the energy, E^* , and either L^* or the impact parameter, b^* . Hence it is convenient to introduce the reduced phase shift^{3a/}

$$\eta^* = \eta / A = \Lambda^* \eta / 2\pi E^{*1/2} \quad (11)$$

Values of this quantity are also tabulated in Table A1.

The dependence of the reduced phase shift, η^* , on the quantum parameter, Λ^* , for $L^{*2} = 1.6$ and a number of values of the energy is illustrated in Figs. 2 and 3. In Fig. 2, the abscissa is ℓ , which according to Eq. 7 is proportional to $1/\Lambda^*$. In Fig. 3, the abscissa is Λ^{*2} . In Fig. 2, as one proceeds to the right (smaller values of Λ^*) the system becomes "more classical"; in Fig. 3 the classical limit is approached at the left.

The existence of the minimum and maximum in ϕ^* implies the existence of a number of quasi-bound or virtual states of positive energy. These are in the energy range between the minimum and maximum of ϕ^* , given, in this case, by Eq. 10. The number of virtual states increases as the system becomes more classical, i.e. as Λ^* becomes smaller. Thus at a fixed value of E^* , a

discrete set of values of Λ^* exists for which this value of E^* is the energy of a virtual state. In the calculations these values of Λ^* are marked by the passage of a node in the radial wave function from the outer classical region, through the potential barrier (the classically forbidden region) into the inner "classical" region, as the value of Λ^* is decreased (at constant E^*). The value of Λ^* at which a node first enters the non-classical region is indicated by a mark on the curves in Figs. 2 and 3. In the neighborhood of each of these values of Λ^* , the phase shift increases by π . This results in a series of maxima in the reduced phase shift, η^* . As the system becomes more classical the maxima occur at smaller intervals in Λ^* and are more "saw tooth" in nature. It is seen from Fig. 3 that at energies below or well above those leading to three turning points, the reduced phase shift approaches a "classical limit" smoothly as $\Lambda^* \rightarrow 0$. At energies in the three turning point range, η^* oscillates with increasing frequency but decreasing amplitude as $\Lambda^* \rightarrow 0$. Nevertheless, a limit apparently exists.

For values of L^* and E^* leading to one classical turning point, the limiting value of η^* is given by the well known first-order JWKB approximation. A more general expansion of the phase shift in powers of Planck's constant applicable to cases in which any (odd) number of turning points occur has been developed^{4/}. The result of this development is that the reduced phase shift is

expanded in powers of Λ^{*2} and may be written

$$\eta^* = \eta^{*(1)} + \Lambda^{*2} \eta^{*(2)} + \dots \quad (12)$$

where

$$\eta^{*(1)} = \lim_{R \rightarrow \infty} \left\{ \int_0^R [1 - \phi^*/E^*]^{\frac{1}{2}} dr^* - \int_0^R [1 - b^{*2}/r^{*2}]^{\frac{1}{2}} dr^* \right\} \quad (13)$$

and

$$\eta^{*(2)} = (96\pi^2 E^*)^{-1} \int_0^R [1 - \phi^*/E^*]^{-\frac{1}{2}} \left[\frac{3}{r^{*2}} - \frac{\phi^{*'''}{\phi^{*'}} - \left(\frac{\phi^{*''}}{\phi^{*'}} \right)^2 \right] dr^* \quad (14)$$

The three integrations are over those regions of r^* for which the integrands are real, i.e. over the "classical" regions. Thus at energies leading to three turning points, $\eta^{*(1)}$ and $\eta^{*(2)}$ each consist of two contributions: one from the integration between the two inner turning points, i.e. the "inner" contribution, $\eta_i^{*(j)}$, and one due to the integration from the outer turning point to infinity, the "outer" contribution, $\eta_o^{*(j)}$. Values of the two contributions to $\eta^{*(1)}$ and $\eta^{*(2)}$ are given in Table 1, for $L^{*2} = 1.6$ and several values of E^* .

It follows from Eq. 12 that $\eta^{*(1)}$ is the reduced phase shift in the classical limit. The numerical values of $\eta^{*(1)}$ given in Table 1 are illustrated in Fig. 4. At energies leading to three

turning points the two separate contributions are illustrated in this figure. The lower curve is the "outer" contribution, $\eta_o^{*(1)}$, and the upper curve is the sum of the "inner" and "outer" contributions, $\eta^{*(1)} = \eta_i^{*(1)} + \eta_o^{*(1)}$.

The solid straight lines in Fig. 3, at energies leading to one turning point, are given by Eq. 7 with the values of $\eta^{*(1)}$ and $\eta^{*(2)}$ given in Table 1. The intercept, $\eta^{*(1)}$, is the usual first order JWKB result. It is seen in this figure, that the deviation of η^* from the horizontal for $E^* = 0.21$ and 0.60 is adequately described by the second order JWKB result, i.e. by the inclusion of $\eta^{*(2)}$. The values of $\eta^{*(1)}$, at energies leading to three turning points, are indicated by arrows on the vertical axis of Fig. 3. These confirm that the limiting value of the reduced phase shift in the three turning point region is indeed $\eta^{*(1)}$, the sum of the contributions from the two classical regions as discussed above.

The sharp sawtooth behavior of η^* as a function of $\sqrt{E^*}$ (or ℓ) in the three turning point region is due primarily to the physically uninteresting inclusion of a number of multiples of π due to the nodes of the radial wave function in the inner region. Let M be the number of nodes of the radial wave function in the inner classical and classically forbidden regions, i.e. the number of quasi-bound or virtual states of energy less than E^* . Thus $M = \nu + 1$, where ν is the vibrational quantum number of the highest quasi-bound state of energy less than E^* . It is then

useful to define a modified phase shift

$$\tilde{\eta}_l = \eta_l - M\pi \quad (15)$$

in which the contribution of the virtual states is excluded. The modified reduced phase shift is then defined as

$$\tilde{\eta}^* = \eta^* - M\pi/A = \eta^* - \frac{\Lambda^* M}{2E^{*1/2}} \quad (16)$$

In Fig. 5, $\tilde{\eta}^*$ is plotted as a function of Λ^{*2} at four values of E^* in the three turning point range. (The small Λ^* portions of these figures, i.e. $\Lambda^{*2} < 0.01$, are enlarged in Figs A 1, 2, and 3 of the Appendix.) At lower values of E^* (i.e. 0.31 and 0.35) most of the oscillatory behavior of η^* (cf. Figs. 2 and 3) is removed by this procedure.

If the second order JWKB contribution to the phase shift were negligible, one might define a "residual" phase shift as

$$\eta_{res}^{(l)} = \tilde{\eta}_l - A \eta_o^{*(l)} \quad (17)$$

where $\eta_o^{*(l)}$ is the "outer" contribution to $\eta^{*(l)}$. In Fig. A 4 of the Appendix, $\eta_{res}^{(l)}$ is plotted as a function of l . The deviation of the mean curve from zero, i.e. the overall trend, is associated with second order (and higher) JWKB contributions.

In order to isolate the sharp rises^{3b/} in the phase shift associated with barrier penetration under resonance conditions, we define a "resonance" contribution to the phase shift,

$$\eta_{res}^{(2)} = \tilde{\eta} - A \left[\eta_o^{*(1)} + \Lambda^{*2} \eta_o^{*(2)} \right] \quad (18)$$

by removing the "outer" contributions to both the first and second order JWKB approximations.

Fig. 6 is a series of plots of $\eta_{res}^{(2)}$ as a function of ℓ at various values of E^* . The "resonance" phase shifts are generally well-behaved and with the exception of $E^* = 0.40$, small in magnitude except near the values of ℓ corresponding to resonance. The curve at $E^* = 0.40$ shows an overall trend from zero since near the broad barrier maximum the second order JWKB approximation is inadequate and the higher order JWKB contributions are significant. (Comparison with the corresponding curve for $\eta_{res}^{(1)}$ in Fig. A 4 indicates that the second-order JWKB term is an over-correction in this case.) Similar considerations apply to the region of small ℓ in which the quantum parameter Λ^* is sufficiently large that the truncated series is no longer adequate.

Analysis of Results

The effect on the phase shift of the tunneling and penetration of the centrifugal barrier has been considered by Ford, Hill, Wakano, and Wheeler^{3b/}. On the basis of a first-order JWKB

approximation, they obtained an expression for the "resonance contribution" to the phase shift. Their expression, valid at energies not too close to the barrier maximum, is (in the present notation):

$$\eta_{res}^{(1)} = \tilde{\eta} - A\eta_0^{*(1)} = \cot^{-1} \left[\cot \left(A\eta_i^{*(1)} - \frac{\pi}{2} \right) - 2e^I \right] \quad (19)$$

where

$$I = A \int [\Phi^*/E^* - 1]^{1/2} dr^* = c(L^*, E^*)/\Lambda^* \quad (20)$$

is the "barrier penetration integral". The integration in this expression is between the two outer turning points, i.e. over the classically forbidden region.

The barrier penetration integral and the constant, $c(L^*, E^*)$, may, of course, be evaluated by direct quadrature. At energies not too far below the barrier maximum, the constant may also be approximated by use of a parabolic approximation for the effective potential, Φ^* . The curvature of Φ^* at the barrier maximum, Φ_{max}^* , is

$$\kappa = \left[d^2 \Phi^*(r^*) / dr^{*2} \right]_{r_{max}^*} \quad (21)$$

and the approximation gives

$$c(L^*, E^*) = \pi^2 \left(\frac{-2}{\mathcal{K}} \right)^{1/2} [\phi_{\max}^* - E^*] \quad (22)$$

Values of $c(L^*, E^*)$ for $L^{*2} = 1.6$, obtained by the two methods, are given in Table 2 for the four "standard" energies of the present study. For this example, $\phi_{\max}^* = 0.400804$ and $\mathcal{K} = 1.5478$. It is seen from the table that in this case the maximum error in the parabolic approximation to the integral is about 17%.

From Eq. 19, it follows that the resonance condition on A is

$$\cot(A_m \eta_i^{*(1)} - \pi/2) = 2e^I \quad (23)$$

where A_m is the value of A leading to the m th resonance ($m = 1, 2, 3, \dots$). If the \cot^{-1} of Eq. 19 is interpreted as the principal value, then as A increases through A_m , $\eta_{res}^{(1)}$ rises to $\pi/2$, falls discontinuously to $-\pi/2$ and begins to rise again. The discontinuous jump of π is associated with the definition of $\tilde{\eta}$, Eq. 15. If in the second equality of Eq. 19, $\tilde{\eta}$ is replaced by η , then the value of the \cot^{-1} must be determined from the continuity of the phase shift.

Let us define

$$M^{(1)} = \frac{1}{2} + \frac{1}{\pi} A \eta_i^{*(1)} = \frac{1}{2} + \frac{2E^{*1/2}}{\Lambda^4} \eta_i^{*(1)} = \frac{1}{2} + \frac{E^{*1/2}}{\pi L^*} \eta_i^{*(1)} (l + \frac{1}{2}) \quad (24)$$

and write the resonance condition, Eq. 23, in the form

$$\tan [\pi (M_m^{(1)} - 1)] = \frac{1}{2} e^{-I} = \frac{1}{2} e^{-c/\Lambda^*} \quad (25)$$

From this form it follows that if Λ^* is sufficiently small the condition of resonance is that $M^{(1)}$ be an integer. From the definition, Eq. 24, this implies that the resonances should be equally spaced in ℓ . This is in qualitative accord with the results shown in Figs. 2 and 6. The arrows on the abscissae of Figs. 5 and 6 denote the values at which $M^{(1)} = 1, 2, 3, \dots$. The values of Λ^{*2} or ℓ at which a node of the radial wave function enters the classically forbidden region, as determined by the direct computations, are indicated by bars (labelled by M) above the axis on Fig. 6. Although the semiclassical results are in fair agreement with the direct quantum results, the discrepancies are not negligible. As an attempt to improve the agreement, a second-order JWKB analogue of $M^{(1)}$ may be defined as

$$M^{(2)} = \frac{1}{2} + \frac{2E^{*k}}{\Lambda^*} [\eta_i^{*(1)} + \Lambda^{*2} \eta_i^{*(2)}] \quad (26)$$

It may then be assumed that the resonance condition is that

$M^{(2)} = 1, 2, 3, \dots$. It is found that this modification improves the prediction of the resonance energies.

The detailed shape of the resonance contribution to the phase

shift is also influenced by the second order JWKB effects. The semi-classical expression for $\eta_{res}^{(1)}$ given by Eq. 19 agrees only qualitatively with the results of the direct quantum calculations given in Fig. A 4 of the Appendix. Empirically, it is found that this equation may be improved considerably by the introduction of second-order JWKB terms. Thus it is postulated that

$$\eta_{res}^{(2)} = \tilde{\eta} - A(\eta_0^{*(1)} + \Lambda^{*2} \eta_0^{*(2)}) = \cot^{-1} \left\{ \cot[\pi(M^{(2)} - 1)] - 2e^I \right\} \quad (27)$$

It is found by comparison with the numerical results of the previous section that although this modification improves the agreement and describes the general features of the resonance phase shifts quite well, it is not quantitatively satisfactory. For example, the quantum calculated curves of $\eta_{res}^{(2)}$ vs. ℓ (see Table A 1 and Fig. 6) are very nearly symmetric about zero (with the exception of the results at very low ℓ and at $E^* \cong \phi_{max}^*$), yet Eq. 27 predicts an asymmetry⁵.

In the preceding discussion, we have considered the resonance structure of the phase shift as Λ^* is varied at fixed values of L^* and E^* . The lifetime of a virtual state and the width of the resonance contribution to the scattering cross section, however, depend on the variation of the phase shift with E^* for fixed values of L^* and Λ^* . In order to investigate these quantities, a number of computations of η_ℓ at closely spaced

values of E^* were carried out. The calculations were made in the regions of the resonances which occurred at the four "standard" energies of the present study. The results of these resonance scans are given in Table 3 and some of the results are illustrated in Fig. 7.

In the neighborhood of each resonance the phase shift as a function of E^* increases more or less abruptly by about π . The "quantum" values of the resonance energy listed in Table 3 are those values of E^* at which a point of inflection (a point of maximum slope) occurs in $\eta_l(E^*)$. The "semi-classical" value of E_{res}^* is that at which $M^{(2)}$ defined by Eq. 26 takes on the higher of the two integer values indicated in the M column of the table. With the exception of the one broad resonance at $E^* = 0.40$, the average error in the predictions of E_{res}^* is 1 part in 3000.

The general problem of predicting resonance energies $E_{res}^*(v, l)$ is of some importance. For a practical system the value of Λ^* is, of course, fixed by the reduced mass and potential constants. At the discrete values of L^* , (given by Eq. 7) corresponding to each of the rotational quantum numbers l , the integrals $\eta_i^{*(0)}$ and $\eta_i^{*(2)}$ are computed as functions of E^* (by Eqs. 13 and 14). The reduced resonance energies $E_{res}^*(v, l)$ are those values of E^* for which the right side of Eq. 26 takes on the integer values $M^{(2)} = v + 1$, where v is the vibrational quantum number.

The maximum slope, $(d\eta_l/dE)_{max}$, is simply related to the level width Γ and the lifetime τ of the virtual state,

$$\left(\frac{d\eta_i}{dE}\right)_{\max} = \frac{2}{\Gamma} = \frac{2\tau}{\hbar} \quad (28)$$

Ford, Hill, Wakano, and Wheeler^[3b] have developed an approximate expression for these quantities^[6]. In the present notation, this is

$$\begin{aligned} \left(\frac{d\eta_i}{dE^*}\right)_{\max} &= \frac{2}{\Gamma^*} = 4 \cdot \left[e^{2c/\Lambda^*} + 1 \right] \frac{d}{dE^*} (A\eta_i^{*(n)}) \\ &= \frac{1}{\Lambda^*} \cdot \left[e^{2c/\Lambda^*} + 1 \right] \cdot F(L^*, E^*) \end{aligned} \quad (29)$$

where

$$F(L^*, E^*) = 8\pi E^{*K_2} \cdot \left[\frac{d\eta_i^{*(n)}}{dE^*} + \frac{\eta_i^{*(n)}}{2E^*} \right]$$

and $\Gamma^* = \Gamma/\epsilon$ is a "reduced" level width. Values of $F(L^*, E^*)$ for the present example are given in Table 4. Values of $(d\eta_i/dE^*)_{\max}$ and Γ^* thus calculated are compared with the results of the direct quantum computations in Table 3; the results are in fair agreement.

The reduced total scattering cross section is

$$Q^* = Q/\pi\sigma^2 = \sum_l Q_l^* \quad (30)$$

where

$$Q_l^* = \frac{4}{A^2} (2l+1) \sin^2 \eta_l = \frac{16 L^{*2}}{(2l+1) E^*} \sin^2 \eta_l \quad (31)$$

is the partial cross section due to the l th phase. In the region of a resonance the corresponding partial cross section varies rapidly with energy, while the remaining contributions to the cross section vary slowly (on the same scale). Fig. 7 illustrates $\eta_l(E^*)$ and the corresponding contribution $Q_l^*(E^*)$ to the reduced total cross section for the three resonances (Table 3) of measurable width.

The partial cross section curves are of the typical resonant shape⁷. If the resonances do not seriously overlap, these shapes should be observable as perturbations on an otherwise smooth background in low energy (i.e., $E^* \lesssim 0.8$) molecular beam scattering measurements. They should be easily distinguishable from the broad, symmetric (positive and negative) undulations in $Q(E)$ for $E^* \gtrsim 0.8$, i.e., the extrema-effect⁸. From the widths and shapes of the resonances it should be possible to infer considerable information about the scattering phase shifts and thus the interaction potential $\phi(r)$.

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Table 1 ^a

| E^* | $\eta_o^{*(1)}$ | $\eta_o^{*(2)}$ | $\eta_i^{*(1)}$ | $\eta_i^{*(2)}$ |
|-------|-----------------|--------------------------|-----------------|-------------------------|
| 0.21 | 0.037795 | 3.914×10^{-3} | | |
| 0.22 | 0.040865 | 4.3647×10^{-3} | 0.00382 | 4.5128×10^{-3} |
| 0.23 | 0.044073 | 4.8695×10^{-3} | 0.01383 | 5.0177×10^{-3} |
| 0.31 | 0.076146 | 1.2887×10^{-2} | 0.09024 | 1.331×10^{-2} |
| 0.35 | 0.098992 | 2.6213×10^{-2} | 0.13048 | 2.675×10^{-2} |
| 0.39 | 0.133686 | 1.3554×10^{-1} | 0.18040 | 1.362×10^{-1} |
| 0.40 | 0.149181 | 1.8281 | 0.19943 | 1.8288 |
| 0.41 | 0.386506 | -3.2096×10^{-1} | | |
| 0.45 | 0.449581 | -7.4293×10^{-2} | | |
| 0.60 | 0.482049 | -2.9742×10^{-2} | | |

^a. Entries refer to the "standard" case of the present study, i.e., an L.-J.(12,6) potential with $L^{*2} = 1.6$.

Table 2

| E^* | $c(1.2649, E^*)$ | |
|-------|-------------------|-------------------------|
| | Parabolic approx. | Quadrature ^a |
| 0.31 | 1.019 | 0.971 |
| 0.35 | 0.570 | 0.514 |
| 0.39 | 0.1212 | 0.104 |
| 0.40 | 0.00903 | 0.008 |

^a From unpublished calculations of P. M. Livingston

Table 3

| l | Λ^* | E_{res}^* | | $(d\eta_l/dE^*)_{\text{res}}$ | | Γ^* | | M |
|-----|-------------|--------------------|------------|-------------------------------|---------------------|----------------------|----------------------|----------------------------------|
| | | Semiclass. Quantum | Quantum | Semiclass. Quantum | Quantum | Semiclass | Quantum | |
| | | | | (Eq. 29) | | | | |
| 118 | 0.0671 | 0.31006 | 0.31005 | 4×10^{15} | $> 3 \times 10^4$ | 5×10^{-16} | $< 6 \times 10^{-5}$ | $1 \rightarrow 2$ |
| 197 | 0.0402 | 0.31011 | 0.31005 | 4×10^{24} | $> 3 \times 10^4$ | 5×10^{-25} | $< 6 \times 10^{-5}$ | $2 \rightarrow 3$ |
| 25 | 0.3117 | 0.34911 | 0.34855 | 2.3×10^3 | 3.2×10^3 | 8.7×10^{-4} | 6.2×10^{-4} | $0 \rightarrow 1$ |
| 77 | 0.1025 | 0.34942 | 0.34935 | 1×10^7 | $> 3 \times 10^4$ | 2×10^{-7} | $< 6 \times 10^{-5}$ | (0.34915) $1 \rightarrow 2$ |
| 128 | 0.0619 | 0.35008 | 0.35005 | 3×10^{10} | $> 3 \times 10^4$ | 1×10^{-10} | $< 6 \times 10^{-5}$ | $2 \rightarrow 3$ |
| 87 | 0.0908 | 0.39010 | 0.39006 | 5.3×10^3 | 4.9×10^3 | 3.8×10^{-4} | 4.1×10^{-4} | $2 \rightarrow 3$ |
| 123 | 0.0643 | 0.38973 | 0.38967 | 2.1×10^4 | $1.4_3 \times 10^4$ | 1.0×10^{-4} | 1.4×10^{-4} | (0.3904) $3 \rightarrow 4$ |
| 137 | 0.0578 | 0.40003 | > 0.4012 | 1.6×10^3 | $> 0.7 \times 10^3$ | 1.3×10^{-3} | $< 3.10^{-3}$ | $4 \rightarrow 5$ |

 ∇ The value of M changes (as indicated) at precisely the listed "quantum" values of E_{res}^* , except in a few cases with a slight difference; this E^* is then listed below the M change (in parentheses).

Table 4F(1.2649, E^{*})

| | | | | |
|----------------|------|------|------|------|
| E [*] | 0.31 | 0.35 | 0.39 | 0.40 |
| F | 15.3 | 18.4 | 31.1 | 38.9 |

APPENDIX

Table A1 (1-7) lists the results of the main body of computations. The column headings have the following meanings (see text for definitions):

| | |
|--------------|--|
| ESTAR | E^* (reduced energy) |
| LAMBDASTAR | Λ^* (quantum parameter) |
| L | ℓ (orbital angular momentum or rotational quantum number) |
| ETA | η (phase shift) |
| ETASTARTILDA | $\tilde{\eta}^*$ (modified reduced phase) |
| ETASTAR | η^* (reduced phase) |
| ETASTARCALC | η^* (calc'd via 2nd-order JWKB) |
| ETARES | $\eta_{res}^{(2)}$ (resonance phase shift) |
| M | M (node index) |
| MU | $M^{(2)}$ (2nd-order JWKB node index) |

Figures A1-3 are "enlarged" graphs of the quantum-computed $\tilde{\eta}^*$ vs. Λ^{*2} for various values of E^* . In addition to the four "standard" E^* 's (cf. Fig. 5), results are presented at $E^* = 0.21, 0.22, 0.41, 0.45$ and 0.60 . The straight lines shown represent the second-order JWKB calculations. Occasionally the quantum points are connected by smooth curves for clarity.

Particular attention is called to Fig. A3, $E^* = 0.41$ ($> \phi_{max}^*$);

it is found that the period of the oscillatory pattern may be well accounted for by the JWKB expression (Eqs. 24 and 25) appropriate for $E^* < \phi_{\max}^*$ with a value of $\eta_i^{*(1)}$ estimated by a short extrapolation of the entries of Table 1 to $E^* = 0.41$.

Fig. A4 is a graph similar to Fig. 6, but with the ordinate $\eta_{\text{res}}^{(1)}$. Most of the asymmetry about the zero line is removed by including the second-order JWKB terms (cf. Fig. 6).

REFERENCES

1. J. O. Hirschfelder, C. F. Curtiss and R. B. Bird, Molecular Theory of Gases and Liquids, John Wiley and Sons, Inc., New York, N.Y., 1954; 2nd printing, 1964.
2. S. Imam-Rahajoe, C. F. Curtiss and R. B. Bernstein, J. Chem. Phys. 42, 530 (1965).
- 3.a) K. W. Ford and J. A. Wheeler, Ann. Phys. (N.Y.) 7, 259 (1959);
b) K. W. Ford, D. L. Hill, M. Wakano and J. A. Wheeler, ibid., 7, 239 (1959).
4. C. F. Curtiss and R. S. Powers, Jr., J. Chem. Phys. 40, 2145 (1964).
5. P. M. Livingston (unpublished) has derived a first-order JWKB expression for η_{res} which predicts symmetric behavior about zero.
- 6.a) See B. C. Eu and J. Ross, J. Chem. Phys. (in press) for related work. (b) Also, note the following papers dealing with the resonance effects on the transport cross sections of atomic hydrogen: R. A. Buckingham and J. W. Fox, Proc. Roy. Soc. A267, 102 (1962); R. A. Buckingham, J. W. Fox and E. Gal, ibid., A284, 237 (1965).
7. See, for example, T. Ohmura, Prog. Theor. Phys. (Japan) Suppl. No. 29, 108 (1964).
8. R. B. Bernstein, J. Chem. Phys. 37, 1880 (1962); 38, 2599 (1963); Science 144, 141 (1964).

LEGENDS FOR FIGURES

1. The reduced effective potential $\phi^*(r^*)$ for $L^{*2} = 1.6$. Shown are a number of values of E^* investigated.
2. Reduced phase η^* as a function of ℓ for various values of E^* , all at constant $\phi^*(r^*)$ with $L^{*2} = 1.6$. The vertical bars on the curves at the four "standard" energies denote values of ℓ at which a node enters the classically forbidden region (see text). Note the oscillatory behavior even for energies $E^* > \phi_{\max}^* = 0.4008$ (the dashed curves).
3. Reduced phase as a function of Λ^{*2} for various values of E^* , all at constant $\phi^*(r^*)$. The vertical bars are as in Fig. 2. The solid straight lines through the quantum-computed points at $E^* = 0.21$ and 0.60 are second-order JWKB calculations. The oscillatory behavior at $E^* = 0.41$ (dashed curve) is to be noted (as in Fig. 2). The arrow on the ordinate scale for $E^* = 0.41$ denotes the first-order JWKB limit $\eta^{*(1)}$; for $E^* = 0.31$ and 0.40 the arrows designate the sum of the inner and outer contributions: $\eta^{*(0)} = \eta_o^{*(1)} + \eta_i^{*(1)}$ (see also Fig. 4). The dotted lines indicate "mean values" of the oscillatory reduced phases.
4. First-order JWKB reduced phases $\eta^{*(1)}$ vs. E^* for the standard $\phi^*(r^*)$ with $L^{*2} = 1.6$. The dashed lines denote the range of E^* in which three turning points exist (Eq. 10). In this region two curves are shown: the lower is $\eta_o^{*(1)}$, the upper is the sum

$\eta_o^{*(1)} + \eta_i^{*(1)}$ (see also Fig. 3). The curve labelled J.-B.

represents the Jeffreys-Born approximation for the reduced phase,

$$\eta^* = 3\pi/8 E^* b^{*5}, \text{ which becomes (for } L^{*2} = 1.6) \text{ simply } \eta^* = 0.3638 E^{*3/2}$$

5. The modified reduced phase $\tilde{\eta}^*$ vs. \mathcal{L}^{*2} for the standard energies.

The solid curves represent the quantum computations. The arrows on the ordinate scales indicate the values of $\eta_o^{*(1)}$. The bars on the abscissa (and occasionally a shaded region reflecting the range of uncertainty) denote positions of the node changes (cf. Fig. 2).

The arrows on the abscissa show the 1st-order JWKB predictions (i.e., \mathcal{L}^{*2} for which $M^{(1)} = \text{integer}$; cf. Eq. 24). The dashed lines for $E^* = 0.39, 0.40$ connect points for which $M^{(1)} = \text{half-integer}$.

6. The resonance phase shift $\eta_{\text{res}}^{(2)}$ vs. \mathcal{L} at the standard energies.

The points are the quantum-computed values, connected by smooth curves. The vertical bars denote the node changes (cf. Figs. 2 and 3), with indices M ; the arrows show the 1st-order JWKB predictions ($M^{(1)} = \text{integer}$) as in Fig. 5. Note the near-zero values of $\eta_{\text{res}}^{(2)}$ except near the resonances (except for $E^* = 0.40$ and at small \mathcal{L} ; see text).

7. Resonance detail for three cases. The upper curve shows

$\eta_{\mathcal{L}}/\pi$ vs. E^* ; the lower one $Q_{\mathcal{L}}^*$ vs. E^* (see Eq. 31). Depending upon the "ambient" value of $\eta_{\mathcal{L}}$ different shapes of resonances in the cross sections are obtained; the minimum in $Q_{\mathcal{L}}^*$ occurs when $\eta_{\mathcal{L}}/\pi$ is integer, which occurs (in general) at an E^* slightly different than E_{res}^* (the position of the inflection in $\eta_{\mathcal{L}}(E^*)$).

The dashed line in Q_{123}^* represents the "ambient" (non-resonant) contribution to the cross section. The "widths" of the resonances are well approximated by Γ^* (Table 3).

A1. Modified reduced phase $\tilde{\eta}^*$ vs. Λ^{*2} for $E^* = 0.21, 0.22$ and 0.31 .

Solid straight lines are second-order JWKB predictions.*

A2. Same as Fig. A1, for $E^* = 0.35, 0.39$ and 0.40 .

A3. Same as Figs. A1 and A2, for $E^* = 0.41, 0.45$ and 0.61 .

A4. Resonance phase shift $\eta_{\text{res}}^{(1)}$ (i.e., first-order JWKB) vs. ℓ at the standard energies. Compare with Fig. 6 (i.e., second-order JWKB approximation).

- - - - -
* The ordinate on the figure for $E^* = 0.22$ labelled 0.04096 should read 0.04086.

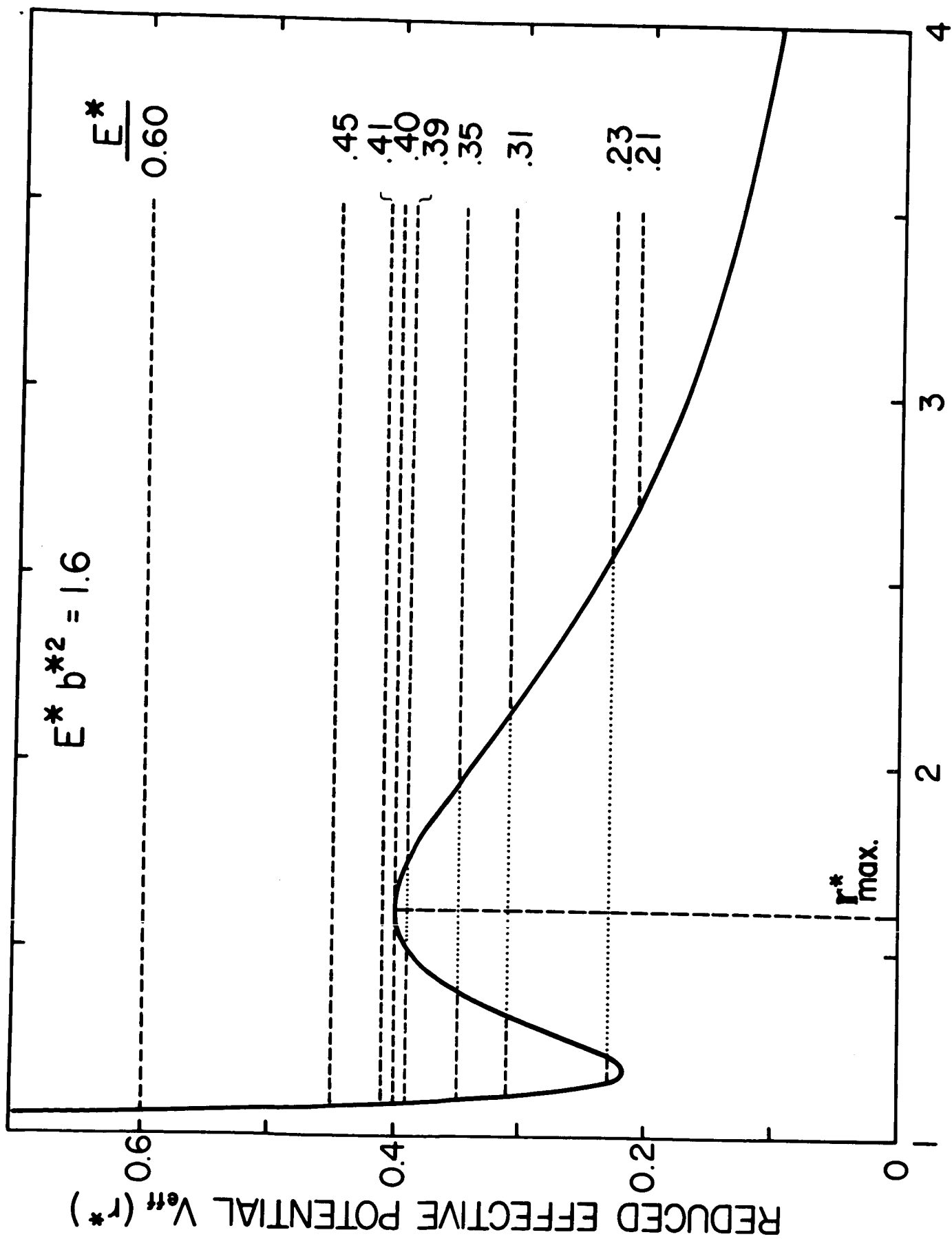


FIGURE 1

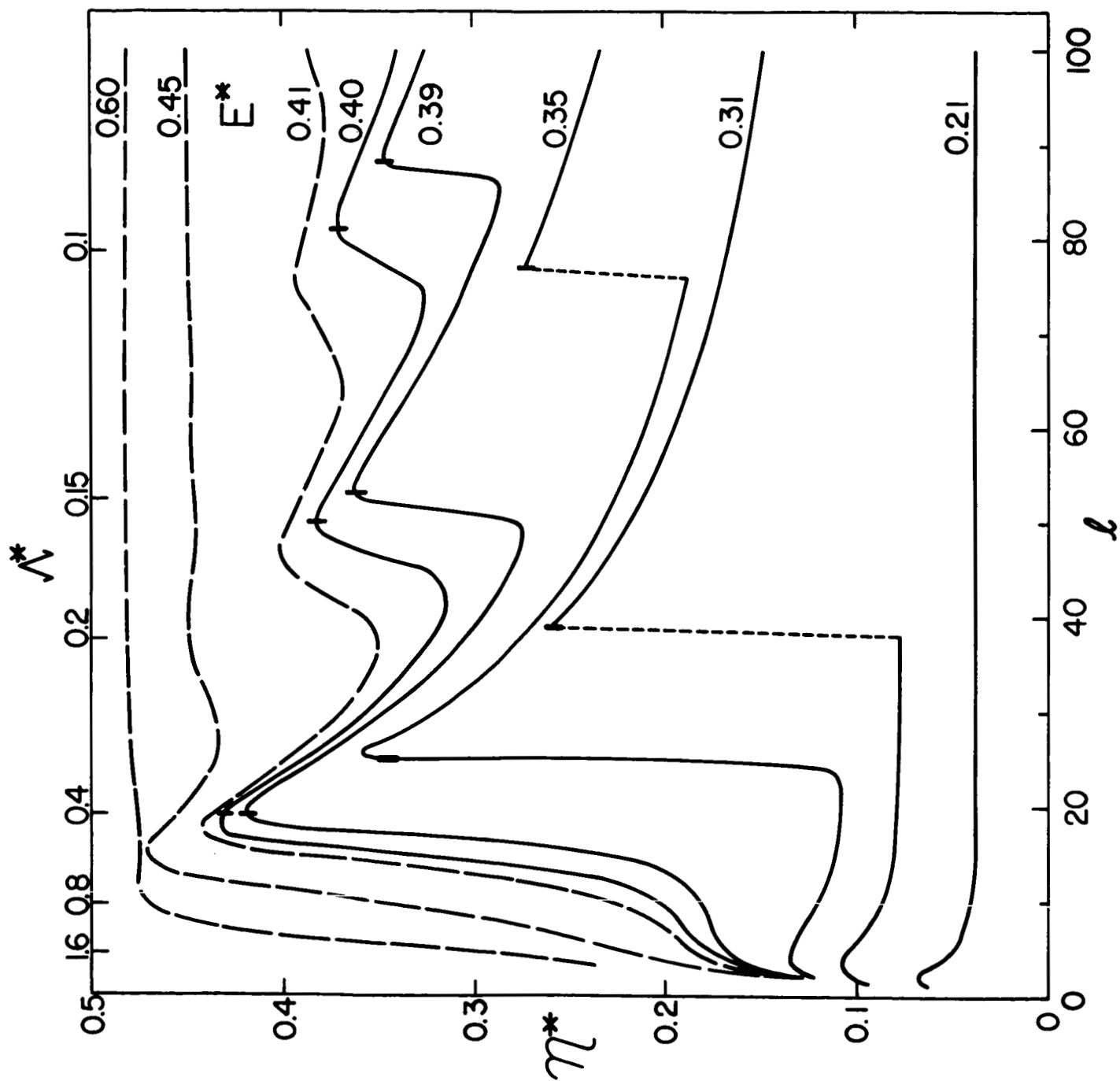


FIGURE 2

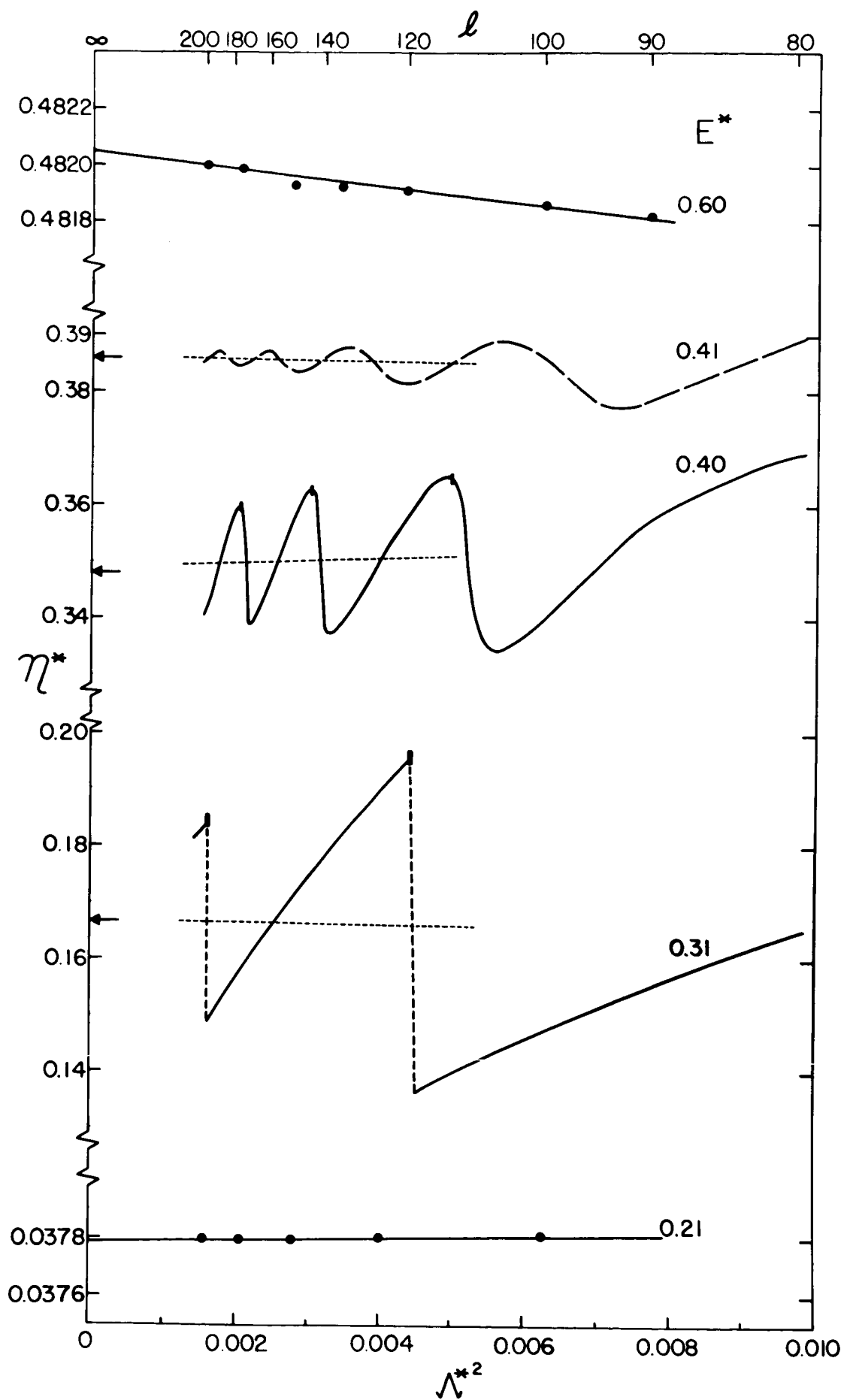


FIGURE 3

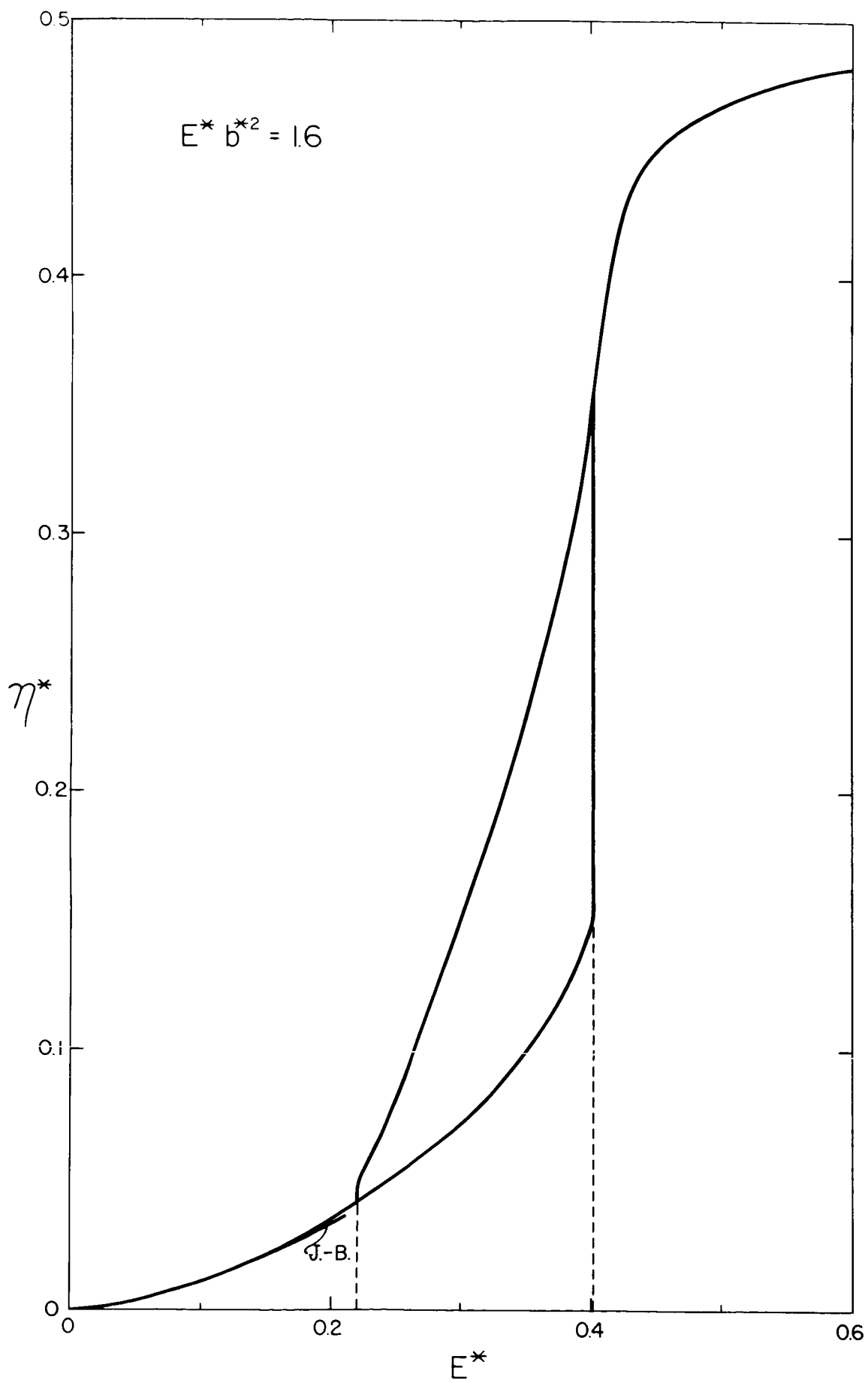


FIGURE 4

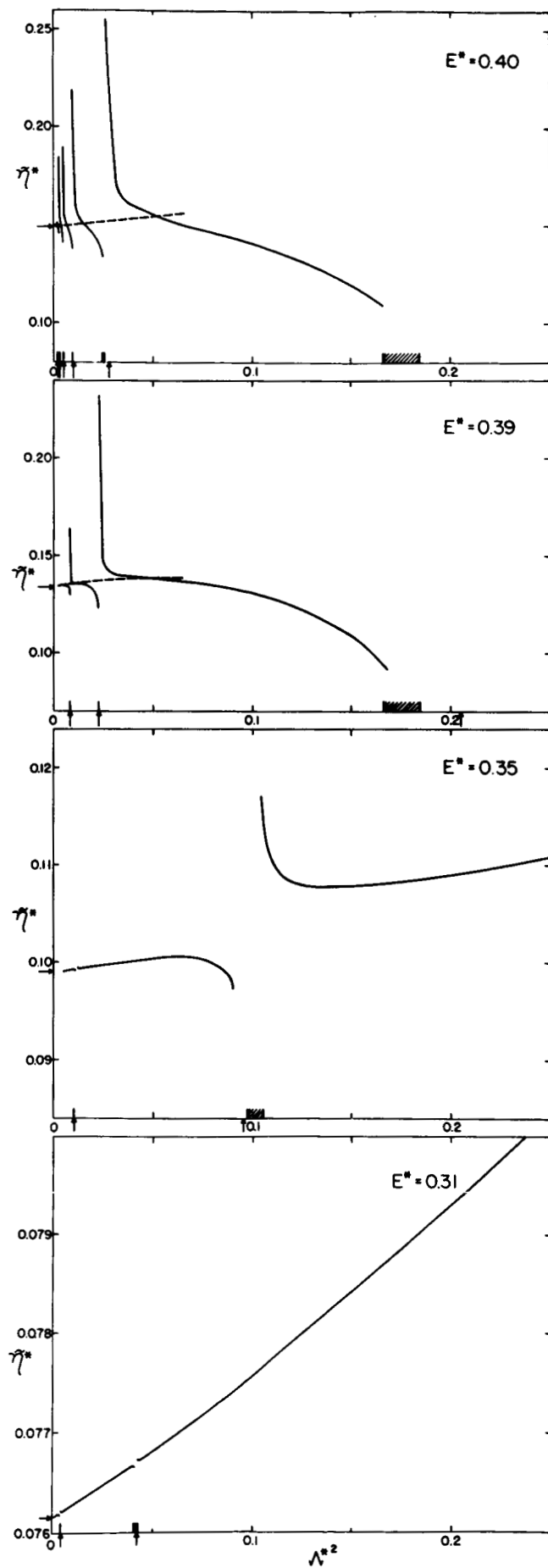


FIGURE 5

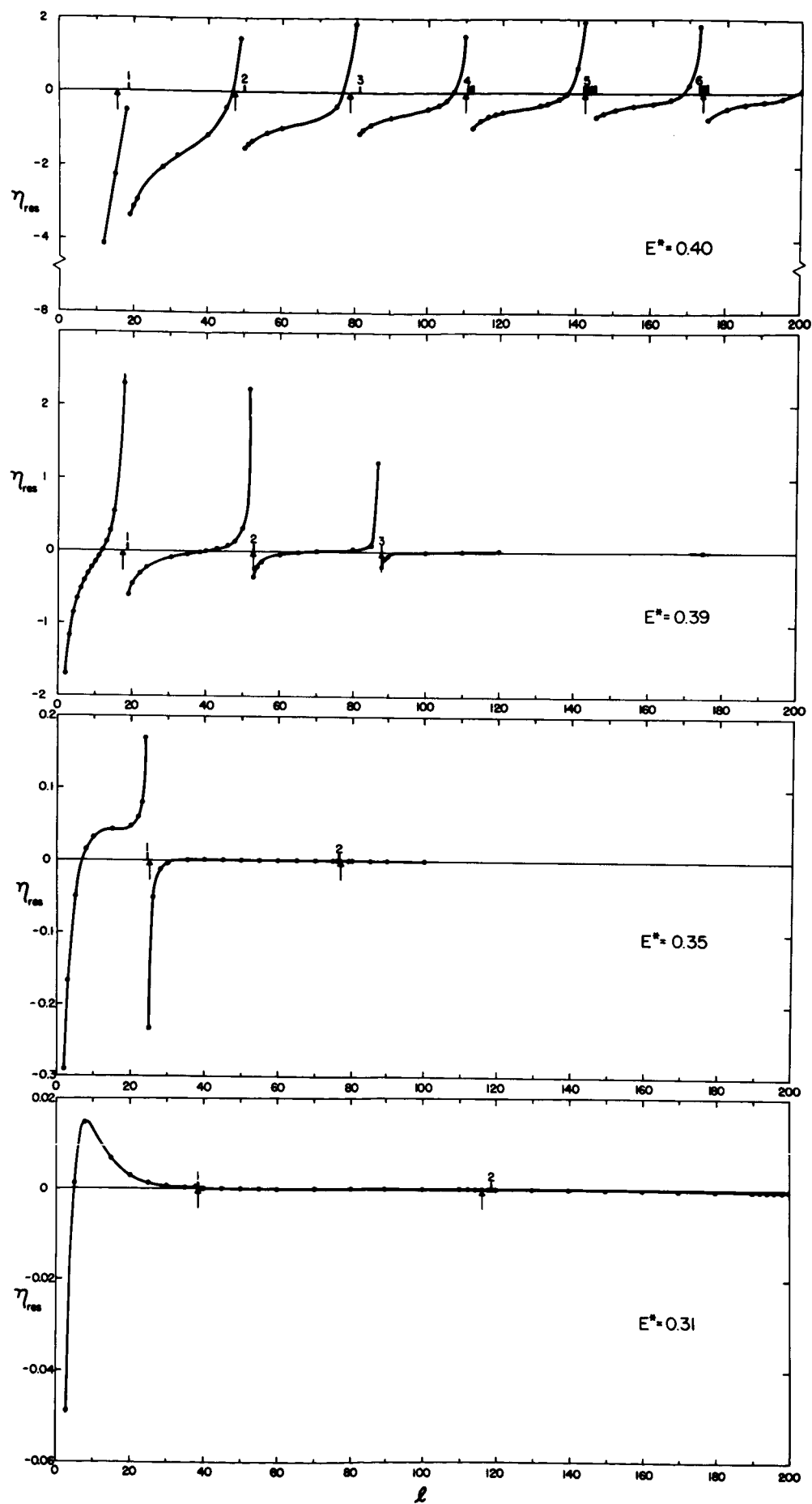


FIGURE 6

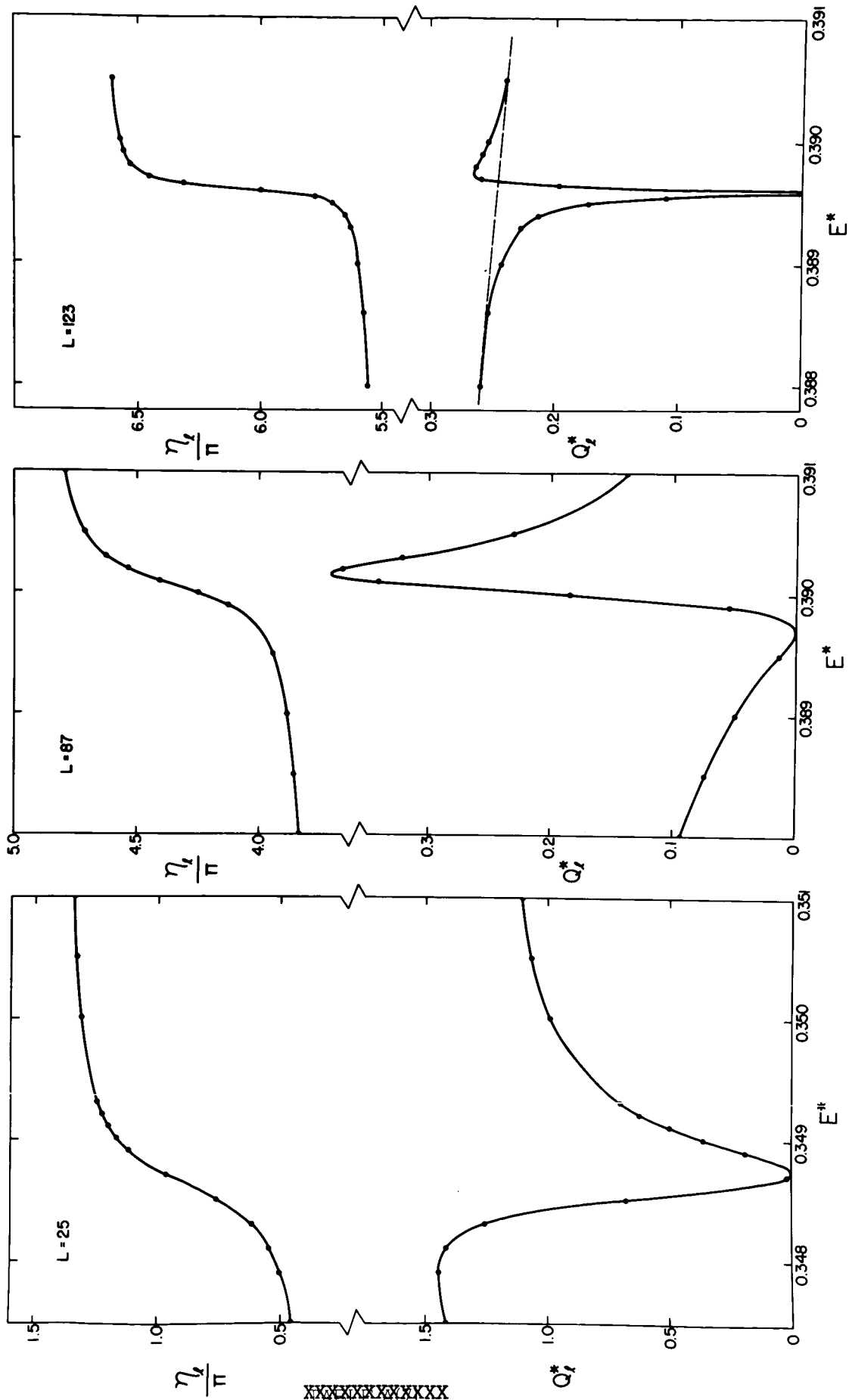


FIGURE 7

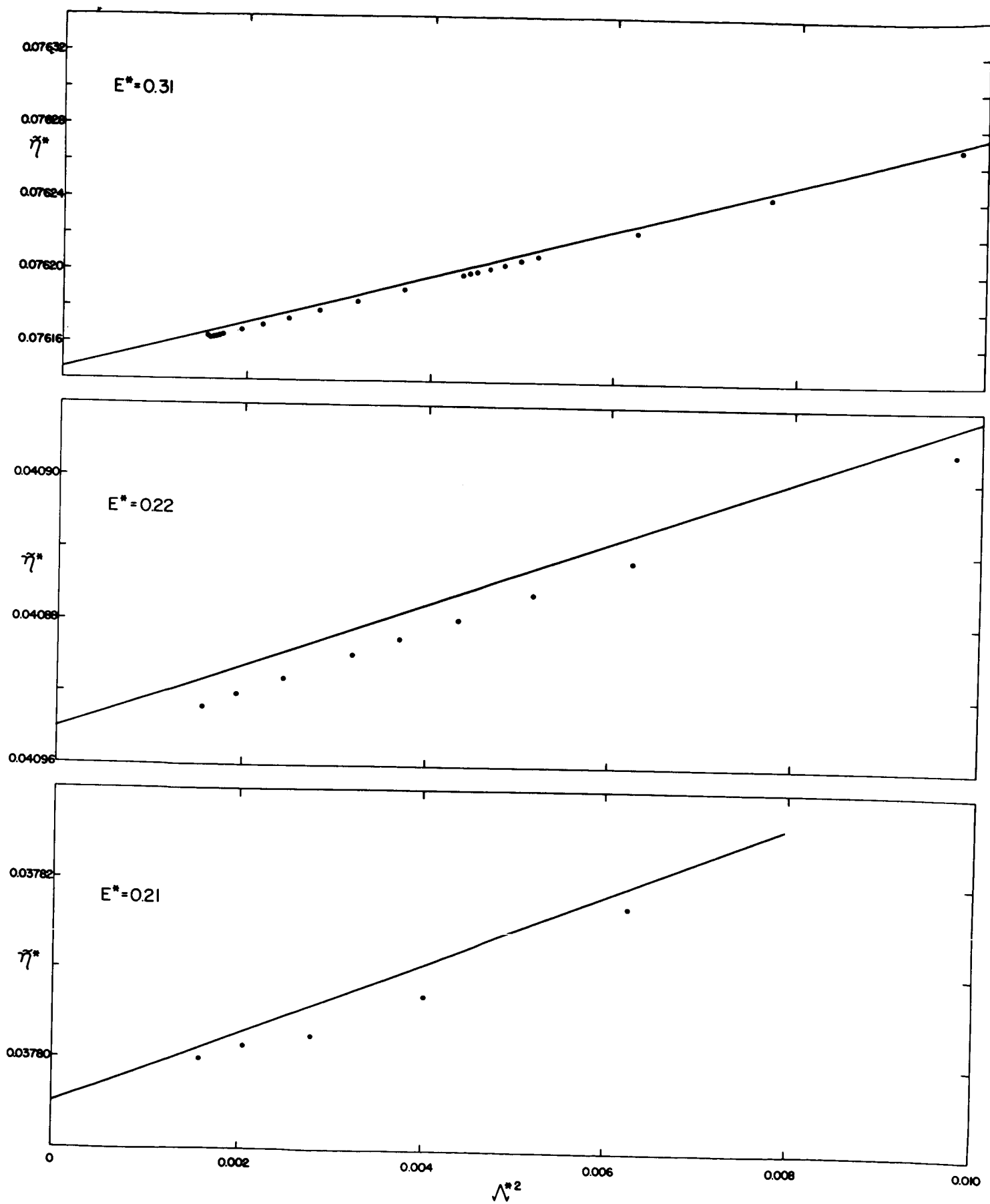


FIGURE A1

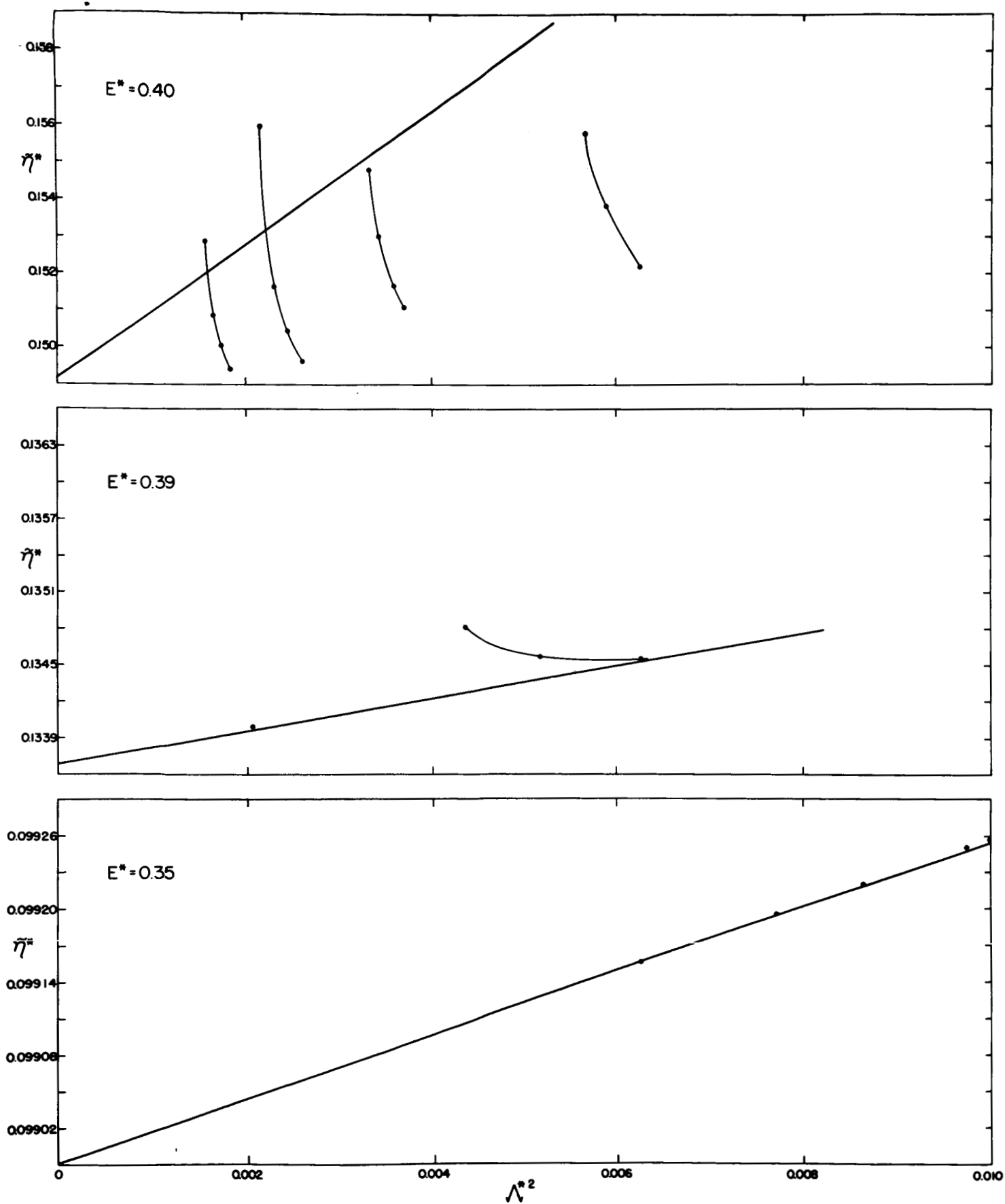


FIGURE A2

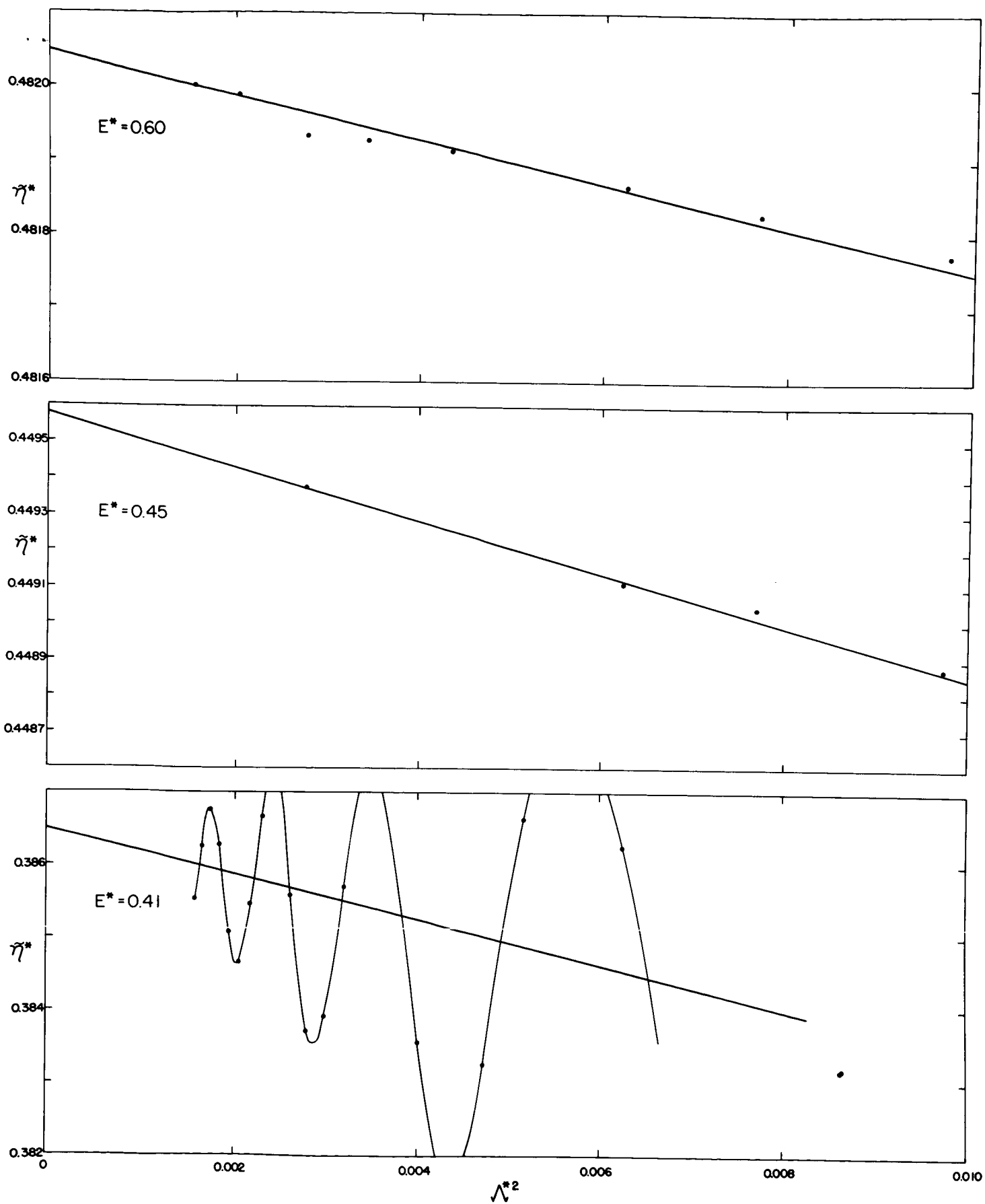


FIGURE A3

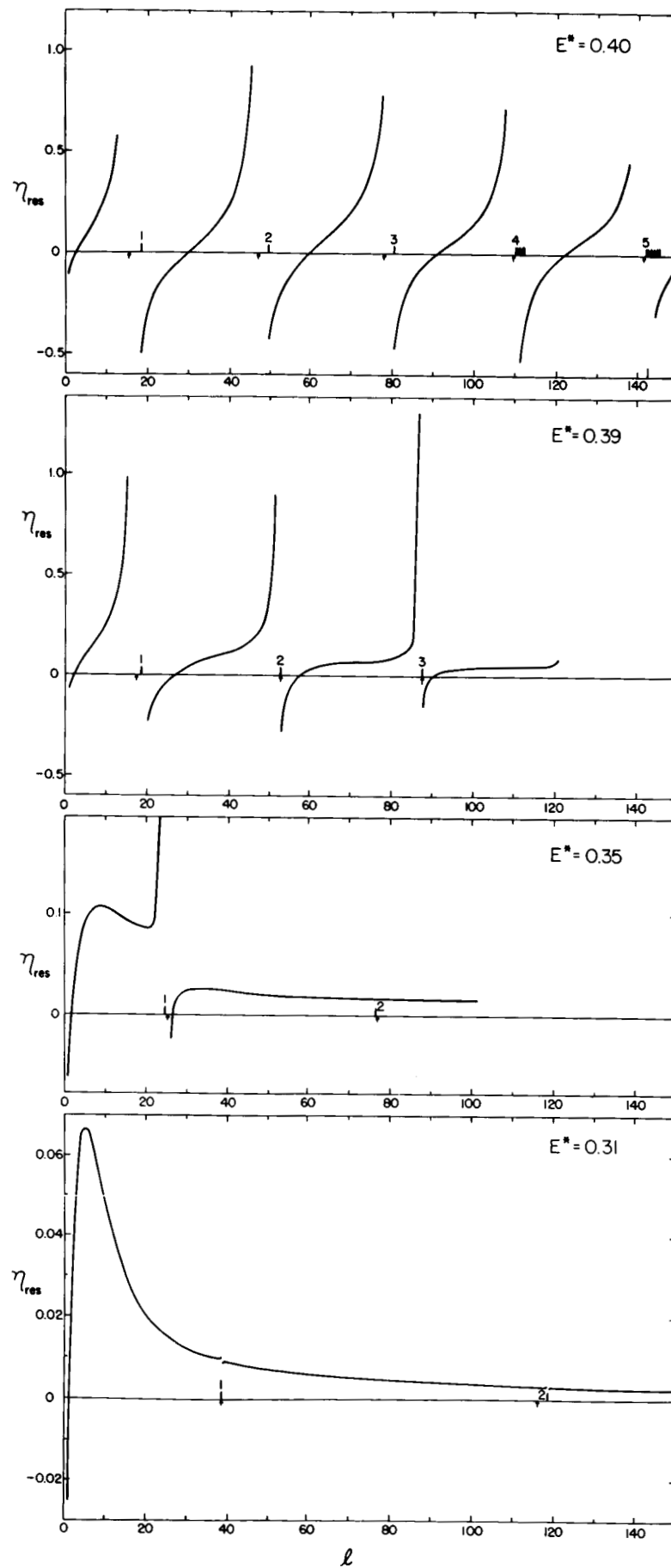


FIGURE A4

ESTAR = .21

| LAMBDASTAR | L | ETA | ETASTARTILDA | ETASTAR | ETASTARCALC | ETARES |
|------------|-----|--------|--------------|---------|-------------|--------|
| 5.2984 | 1 | .0212 | .038997 | .038997 | .147676 | .0591 |
| 3.1791 | 2 | .0617 | .068083 | .068083 | .077352 | .0084 |
| 2.2708 | 3 | .0779 | .061441 | .061441 | .057977 | .0044 |
| 1.4450 | 5 | .0970 | .048706 | .048706 | .045968 | .0055 |
| .7569 | 10 | .1534 | .040316 | .040316 | .040037 | .0011 |
| .3877 | 20 | .2852 | .038398 | .038398 | .038383 | .0001 |
| .2606 | 30 | .4206 | .038062 | .038062 | .038061 | .0000 |
| .1962 | 40 | .5568 | .037946 | .037946 | .037946 | .0000 |
| .1574 | 50 | .6932 | .037890 | .037890 | .037892 | .0000 |
| .0791 | 100 | 1.3769 | .037817 | .037817 | .037819 | .0001 |
| .0653 | 125 | 1.7190 | .037807 | .037807 | .037811 | .0002 |
| .0528 | 150 | 2.0611 | .037803 | .037803 | .037806 | .0002 |
| .0453 | 175 | 2.4034 | .037801 | .037801 | .037803 | .0001 |
| .0396 | 200 | 2.7457 | .037800 | .037800 | .037801 | .0001 |

ESTAR = .22

| LAMBDASTAR | L | M | ETA | ETASTARTILDA | ETASTAR | ETASTARCALC | MU | ETARES |
|------------|-----|---|--------|--------------|---------|-------------|------|--------|
| 5.2984 | 1 | 0 | .0220 | .039593 | .039593 | .163397 | .523 | -.0689 |
| 2.2708 | 3 | 0 | .0857 | .066032 | .066032 | .063371 | .511 | .0035 |
| 1.4450 | 5 | 0 | .1081 | .053005 | .053005 | .049979 | .509 | .0062 |
| .7569 | 10 | 0 | .1702 | .043713 | .043713 | .043366 | .508 | .0014 |
| .3877 | 20 | 0 | .3158 | .041538 | .041538 | .041521 | .511 | .0001 |
| .2606 | 30 | 0 | .4655 | .041162 | .041162 | .041161 | .515 | .0000 |
| .1747 | 45 | 0 | .6917 | .040995 | .040995 | .040998 | .521 | -.0000 |
| .1314 | 60 | 0 | .9184 | .040937 | .040937 | .040940 | .528 | -.0001 |
| .0987 | 80 | 0 | 1.2210 | .040904 | .040904 | .040908 | .537 | -.0001 |
| .0791 | 100 | 0 | 1.5238 | .040889 | .040889 | .040892 | .546 | -.0001 |
| .0719 | 110 | 0 | 1.6752 | .040884 | .040884 | .040888 | .550 | -.0001 |
| .0660 | 120 | 0 | 1.8266 | .040880 | .040880 | .040884 | .555 | -.0002 |
| .0609 | 130 | 0 | 1.9781 | .040878 | .040878 | .040881 | .559 | -.0002 |
| .0566 | 140 | 0 | 2.1296 | .040875 | .040875 | .040879 | .564 | -.0002 |
| .0495 | 160 | 0 | 2.4325 | .040872 | .040872 | .040876 | .573 | -.0002 |
| .0440 | 180 | 0 | 2.7355 | .040870 | .040870 | .040873 | .582 | -.0002 |
| .0396 | 200 | 0 | 3.0384 | .040868 | .040868 | .040872 | .591 | -.0003 |

TABLE A(1)

ESTAR = .31

| LAMBDA STAR | L | M | ETA | ETASTARTILDA | ETASTAR | ETASTARCALC | MU | ETARES |
|-------------|-----|---|---------|--------------|---------|-------------|-------|--------|
| 5.2984 | 1 | 0 | .0278 | .042172 | .042172 | .437930 | .597 | -.2613 |
| 3.1791 | 2 | 0 | .1136 | .103204 | .103204 | .206387 | .579 | -.1135 |
| 2.2708 | 3 | 0 | .1710 | .111024 | .111024 | .142596 | .578 | -.0486 |
| 1.4450 | 5 | 0 | .2507 | .103573 | .103573 | .103056 | .591 | .0013 |
| .9350 | 8 | 0 | .3419 | .091378 | .091378 | .087412 | .621 | .0148 |
| .5128 | 15 | 0 | .5494 | .080529 | .080529 | .079534 | .704 | .0068 |
| .3877 | 20 | 0 | .7076 | .078416 | .078416 | .078083 | .765 | .0030 |
| .3117 | 25 | 0 | .8701 | .077521 | .077521 | .077398 | .827 | .0014 |
| .2606 | 30 | 0 | 1.0347 | .077073 | .077073 | .077021 | .889 | .0007 |
| .2239 | 35 | 0 | 1.2003 | .076817 | .076817 | .076792 | .952 | .0004 |
| .2064 | 38 | 0 | 1.3001 | .076717 | .076717 | .076695 | .990 | .0004 |
| .2012 | 39 | 1 | 4.4744 | .076659 | .257348 | .257357 | 1.002 | -.0002 |
| .1962 | 40 | 1 | 4.5080 | .076650 | .252878 | .252870 | 1.015 | .0001 |
| .1747 | 45 | 1 | 4.6746 | .076545 | .233407 | .233401 | 1.078 | .0001 |
| .1574 | 50 | 1 | 4.8414 | .076468 | .217799 | .217796 | 1.141 | .0001 |
| .1432 | 55 | 1 | 5.0083 | .076411 | .205010 | .205009 | 1.204 | .0000 |
| .1314 | 60 | 1 | 5.1753 | .076368 | .194339 | .194339 | 1.267 | .0000 |
| .1127 | 70 | 1 | 5.5096 | .076309 | .177546 | .177547 | 1.393 | -.0000 |
| .0987 | 80 | 1 | 5.8441 | .076270 | .164931 | .164933 | 1.519 | -.0001 |
| .0878 | 90 | 1 | 6.1787 | .076242 | .155107 | .155110 | 1.646 | -.0001 |
| .0791 | 100 | 1 | 6.5135 | .076223 | .147240 | .147244 | 1.772 | -.0002 |
| .0719 | 110 | 1 | 6.8483 | .076209 | .140800 | .140803 | 1.898 | -.0002 |
| .0706 | 112 | 1 | 6.9153 | .076207 | .139649 | .139652 | 1.923 | -.0002 |
| .0694 | 114 | 1 | 6.9823 | .076205 | .138538 | .138542 | 1.949 | -.0002 |
| .0682 | 116 | 1 | 7.0493 | .076203 | .137466 | .137470 | 1.974 | -.0002 |
| .0671 | 118 | 1 | 7.1162 | .076201 | .136430 | .136434 | 1.999 | -.0002 |
| .0665 | 119 | 2 | 10.2913 | .076199 | .195651 | .195654 | 2.012 | -.0002 |
| .0660 | 120 | 2 | 10.3248 | .076199 | .194659 | .194662 | 2.025 | -.0002 |
| .0609 | 130 | 2 | 10.6597 | .076190 | .185573 | .185576 | 2.151 | -.0002 |
| .0566 | 140 | 2 | 10.9947 | .076184 | .177781 | .177785 | 2.277 | -.0002 |
| .0528 | 150 | 2 | 11.3297 | .076178 | .171025 | .171029 | 2.404 | -.0002 |
| .0495 | 160 | 2 | 11.6647 | .076174 | .165111 | .165115 | 2.530 | -.0003 |
| .0466 | 170 | 2 | 11.9997 | .076170 | .159891 | .159895 | 2.656 | -.0003 |
| .0440 | 180 | 2 | 12.3347 | .076167 | .155250 | .155254 | 2.783 | -.0003 |
| .0417 | 190 | 2 | 12.6698 | .076165 | .151096 | .151100 | 2.909 | -.0003 |
| .0413 | 192 | 2 | 12.7368 | .076164 | .150317 | .150321 | 2.935 | -.0003 |
| .0409 | 194 | 2 | 12.8038 | .076164 | .149554 | .149558 | 2.960 | -.0003 |
| .0404 | 196 | 2 | 12.8708 | .076163 | .148807 | .148811 | 2.985 | -.0003 |
| .0400 | 198 | 3 | 16.0794 | .076163 | .184030 | .184034 | 3.010 | -.0003 |
| .0396 | 200 | 3 | 16.1466 | .076164 | .182955 | .182958 | 3.036 | -.0002 |

TABLE A(2)

ESTAR = .35

| LAMBDA STAR | L | M | ETA | ETASTARTILDA | ETASTAR | ETASTAR CALC | MU | ETARES |
|-------------|-----|---|---------|--------------|---------|--------------|-------|--------|
| 5.2984 | 1 | 0 | .0295 | .042014 | .042014 | .834884 | .697 | -.5562 |
| 3.1791 | 2 | 0 | .1351 | .115543 | .115543 | .363913 | .649 | -.2904 |
| 2.2708 | 3 | 0 | .2162 | .132083 | .132083 | .234156 | .640 | -.1671 |
| 1.4450 | 5 | 0 | .3447 | .133992 | .133992 | .153728 | .653 | -.0508 |
| .9350 | 8 | 0 | .4994 | .125631 | .125631 | .121909 | .695 | .0148 |
| .7569 | 10 | 0 | .5915 | .120455 | .120455 | .114010 | .728 | .0316 |
| .5128 | 15 | 0 | .8103 | .111772 | .111772 | .105884 | .817 | .0427 |
| .3877 | 20 | 0 | 1.0341 | .107851 | .107851 | .102932 | .910 | .0472 |
| .3532 | 22 | 0 | 1.1358 | .107930 | .107930 | .102263 | .948 | .0596 |
| .3382 | 23 | 0 | 1.2011 | .109279 | .109279 | .101990 | .967 | .0801 |
| .3244 | 24 | 0 | 1.3349 | .116496 | .116496 | .101750 | .986 | .1690 |
| .3117 | 25 | 1 | 4.1198 | .082017 | .345429 | .364950 | 1.005 | -.2328 |
| .2999 | 26 | 1 | 4.3470 | .097258 | .350731 | .354822 | 1.024 | -.0507 |
| .2789 | 28 | 1 | 4.4763 | .100130 | .335814 | .336715 | 1.062 | -.0120 |
| .2606 | 30 | 1 | 4.5756 | .100523 | .320753 | .321002 | 1.101 | -.0035 |
| .2239 | 35 | 1 | 4.8081 | .100369 | .289581 | .289517 | 1.197 | .0011 |
| .1962 | 40 | 1 | 5.0373 | .100077 | .265929 | .265853 | 1.293 | .0014 |
| .1747 | 45 | 1 | 5.2664 | .099846 | .247472 | .247418 | 1.389 | .0011 |
| .1574 | 50 | 1 | 5.4959 | .099678 | .232688 | .232651 | 1.486 | .0009 |
| .1432 | 55 | 1 | 5.7258 | .099553 | .220580 | .220557 | 1.583 | .0006 |
| .1314 | 60 | 1 | 5.9559 | .099460 | .210485 | .210469 | 1.679 | .0004 |
| .1213 | 65 | 1 | 6.1863 | .099388 | .201938 | .201928 | 1.776 | .0003 |
| .1127 | 70 | 1 | 6.4169 | .099332 | .194609 | .194602 | 1.873 | .0002 |
| .1053 | 75 | 1 | 6.6476 | .099288 | .188255 | .188249 | 1.970 | .0002 |
| .1039 | 76 | 1 | 6.6938 | .099281 | .187085 | .187079 | 1.989 | .0002 |
| .1026 | 77 | 2 | 9.8814 | .099269 | .272611 | .272610 | 2.009 | .0001 |
| .1000 | 79 | 2 | 9.9738 | .099257 | .268238 | .268235 | 2.047 | .0001 |
| .0987 | 80 | 2 | 10.0200 | .099250 | .266132 | .266130 | 2.067 | .0001 |
| .0930 | 85 | 2 | 10.2509 | .099220 | .256343 | .256342 | 2.164 | .0001 |
| .0878 | 90 | 2 | 10.4819 | .099195 | .247637 | .247636 | 2.261 | .0000 |
| .0791 | 100 | 2 | 10.9439 | .099155 | .232827 | .232828 | 2.455 | -.0000 |

TABLE A(3)

ESTAR = .39

| LAMBDASTAR | L | M | ETA | ETASTARTILDA | ETASTAR | ETASTARCALC | MU | ETARES |
|------------|-----|---|---------|--------------|---------|-------------|-------|---------|
| 5.2984 | 1 | 0 | .0305 | .041247 | .041247 | 3.938773 | 1.444 | -2.8864 |
| 3.1791 | 2 | 0 | .1563 | .126636 | .126636 | 1.503518 | 1.112 | -1.6995 |
| 2.2708 | 3 | 0 | .2642 | .152900 | .152900 | .832580 | .986 | -1.1745 |
| 1.7661 | 4 | 0 | .3641 | .163863 | .163863 | .556473 | .928 | -.8723 |
| 1.4450 | 5 | 0 | .4599 | .169352 | .169352 | .416709 | .902 | -.6717 |
| 1.2227 | 6 | 0 | .5538 | .172586 | .172586 | .336324 | .892 | -.5255 |
| 1.0597 | 7 | 0 | .6475 | .174878 | .174878 | .285890 | .893 | -.4111 |
| .9350 | 8 | 0 | .7424 | .176896 | .176896 | .252184 | .900 | -.3159 |
| .8366 | 9 | 0 | .8398 | .179062 | .179062 | .228550 | .912 | -.2321 |
| .7569 | 10 | 0 | .9422 | .181747 | .181747 | .211341 | .926 | -.1534 |
| .6911 | 11 | 0 | 1.0526 | .185395 | .185395 | .198423 | .944 | -.0740 |
| .6358 | 12 | 0 | 1.1769 | .190708 | .190708 | .188479 | .963 | .0138 |
| .5887 | 13 | 0 | 1.3262 | .198983 | .198983 | .180663 | .983 | .1221 |
| .5461 | 14 | 0 | 1.5251 | .213035 | .213035 | .174406 | 1.004 | .2765 |
| .5128 | 15 | 0 | 1.8345 | .239729 | .239729 | .169322 | 1.027 | .5388 |
| .4296 | 18 | 0 | 3.7397 | .409445 | .409445 | .158701 | 1.098 | 2.2902 |
| .4076 | 19 | 1 | 4.0460 | .093937 | .420257 | .482521 | 1.122 | -.5994 |
| .3877 | 20 | 1 | 4.2416 | .108688 | .419089 | .464460 | 1.147 | -.4592 |
| .3532 | 22 | 1 | 4.5069 | .122908 | .405718 | .433408 | 1.198 | -.3076 |
| .3244 | 24 | 1 | 4.7074 | .129445 | .389169 | .407673 | 1.250 | -.2238 |
| .2606 | 30 | 1 | 5.1974 | .136523 | .345153 | .351520 | 1.409 | -.0959 |
| .2239 | 35 | 1 | 5.5664 | .138352 | .317597 | .319725 | 1.545 | -.0373 |
| .2064 | 38 | 1 | 5.7832 | .138976 | .304254 | .304741 | 1.627 | -.0092 |
| .1962 | 40 | 1 | 5.9279 | .139348 | .296464 | .296022 | 1.682 | .0088 |
| .1827 | 43 | 1 | 6.1486 | .140013 | .286294 | .284492 | 1.764 | .0387 |
| .1709 | 46 | 1 | 6.3841 | .141237 | .278081 | .274489 | 1.847 | .0825 |
| .1639 | 48 | 1 | 6.5697 | .143166 | .274367 | .268526 | 1.903 | .1398 |
| .1574 | 50 | 1 | 6.8745 | .149722 | .275726 | .263048 | 1.958 | .3161 |
| .1514 | 52 | 1 | 8.9076 | .222457 | .343662 | .257997 | 2.014 | 2.2204 |
| .1486 | 53 | 2 | 9.5422 | .123385 | .361263 | .374555 | 2.042 | -.3511 |
| .1458 | 54 | 2 | 9.7530 | .128957 | .362470 | .370081 | 2.070 | -.2048 |
| .1432 | 55 | 2 | 9.8819 | .131337 | .360642 | .365771 | 2.098 | -.1405 |
| .1314 | 60 | 2 | 10.3047 | .134637 | .344992 | .346380 | 2.238 | -.0414 |
| .1213 | 65 | 2 | 10.6591 | .135320 | .329616 | .329979 | 2.378 | -.0117 |
| .1127 | 70 | 2 | 11.0009 | .135542 | .316059 | .315926 | 2.518 | .0046 |
| .0987 | 80 | 2 | 11.6822 | .135846 | .293939 | .293100 | 2.799 | .0333 |
| .0930 | 85 | 2 | 12.0756 | .137220 | .286068 | .283705 | 2.940 | .0997 |
| .0908 | 87 | 2 | 13.3414 | .163387 | .308832 | .280249 | 2.996 | 1.2348 |
| .0898 | 88 | 3 | 15.1302 | .130579 | .346282 | .350482 | 3.024 | -.1835 |
| .0888 | 89 | 3 | 15.2963 | .132880 | .346172 | .348047 | 3.052 | -.0829 |
| .0878 | 90 | 3 | 15.3946 | .133610 | .344546 | .345667 | 3.081 | -.0501 |
| .0791 | 100 | 3 | 16.1012 | .134558 | .324505 | .324481 | 3.363 | .0012 |
| .0719 | 110 | 3 | 16.7662 | .134570 | .307327 | .307145 | 3.645 | .0100 |
| .0660 | 120 | 3 | 17.4451 | .134613 | .293234 | .292696 | 3.927 | .0320 |
| .0453 | 175 | 5 | 27.3178 | .133991 | .315280 | .315253 | 5.483 | .0023 |

TABLE A(4)

| LAMBDA STAR | L | M | ETA | ETASTARTILDA | ETASTAR | ETASTARCALC | MU | ETARES |
|-------------|-----|---|---------|--------------|---------|-------------|--------|----------|
| 5.2984 | 1 | 0 | .0307 | .040942 | .040942 | 51.470423 | 12.804 | -38.5721 |
| 5.1791 | 2 | 0 | .1615 | .129196 | .129196 | 18.624827 | 7.933 | -23.1195 |
| 2.2708 | 3 | 0 | .2765 | .157994 | .157994 | 9.575531 | 5.864 | -16.4807 |
| 1.4450 | 5 | 0 | .4918 | .178845 | .178845 | 3.966463 | 4.017 | -10.4160 |
| 1.0597 | 7 | 0 | .7069 | .188518 | .188518 | 2.202031 | 3.189 | -7.5507 |
| .7569 | 10 | 0 | 1.0757 | .204892 | .204892 | 1.196553 | 2.584 | -5.2062 |
| .6358 | 12 | 0 | 1.4162 | .226588 | .226588 | .888207 | 2.368 | -4.1351 |
| .5128 | 15 | 0 | 2.6268 | .338945 | .338945 | .629817 | 2.178 | -2.2543 |
| .4296 | 18 | 0 | 3.9981 | .432233 | .432233 | .486574 | 2.081 | -.5027 |
| .4076 | 19 | 1 | 4.2061 | .109181 | .431396 | .775072 | 2.062 | -3.3508 |
| .3877 | 20 | 1 | 4.3685 | .119703 | .426200 | .730450 | 2.048 | -3.1186 |
| .3697 | 21 | 1 | 4.5059 | .126915 | .419156 | .691228 | 2.038 | -2.9248 |
| .3532 | 22 | 1 | 4.7987 | .147301 | .426553 | .656528 | 2.031 | -2.5872 |
| .3117 | 25 | 1 | 5.1357 | .156402 | .402802 | .573163 | 2.030 | -2.1721 |
| .2789 | 28 | 1 | 5.2360 | .146975 | .367438 | .511808 | 2.050 | -2.0573 |
| .2445 | 32 | 1 | 5.6051 | .151602 | .344931 | .451833 | 2.097 | -1.7372 |
| .1962 | 40 | 1 | 6.3977 | .160797 | .315937 | .374721 | 2.239 | -1.1904 |
| .1747 | 45 | 1 | 7.3832 | .186446 | .324538 | .343050 | 2.348 | -.4211 |
| .1606 | 49 | 1 | 9.4440 | .254644 | .381577 | .323241 | 2.443 | 1.4438 |
| .1574 | 50 | 2 | 9.6658 | .133966 | .382805 | .443299 | 2.467 | -1.5275 |
| .1543 | 51 | 2 | 9.8343 | .137906 | .381913 | .436726 | 2.492 | -1.4114 |
| .1514 | 52 | 2 | 9.9740 | .140602 | .379962 | .430435 | 2.517 | -1.3249 |
| .1407 | 56 | 2 | 10.4153 | .146271 | .368684 | .407768 | 2.619 | -1.1041 |
| .1314 | 60 | 2 | 10.7926 | .149071 | .356779 | .388437 | 2.724 | -.9577 |
| .1053 | 75 | 2 | 12.3190 | .159889 | .326331 | .335881 | 3.140 | -.3605 |
| .0987 | 80 | 2 | 14.8516 | .212879 | .368983 | .323104 | 3.283 | 1.8466 |
| .0975 | 81 | 3 | 15.1022 | .139323 | .370606 | .397848 | 3.312 | -1.1101 |
| .0963 | 82 | 3 | 15.2834 | .142027 | .370506 | .394626 | 3.341 | -.9950 |
| .0941 | 84 | 3 | 15.5550 | .145095 | .368167 | .388425 | 3.400 | -.8559 |
| .0878 | 90 | 3 | 16.1599 | .148843 | .357125 | .371562 | 3.576 | -.6533 |
| .0791 | 100 | 3 | 17.0729 | .152201 | .339759 | .348171 | 3.873 | -.4227 |
| .0768 | 103 | 3 | 17.3856 | .153833 | .335954 | .342082 | 3.963 | -.3171 |
| .0753 | 105 | 3 | 17.6442 | .155818 | .334487 | .338224 | 4.023 | -.1972 |
| .0739 | 107 | 3 | 18.0391 | .160267 | .335612 | .334518 | 4.083 | .0588 |
| .0719 | 110 | 3 | 19.7297 | .186515 | .357099 | .329222 | 4.174 | 1.5402 |
| .0706 | 112 | 4 | 20.5238 | .141465 | .364868 | .381707 | 4.234 | -.9472 |
| .0694 | 114 | 4 | 20.8784 | .145189 | .364689 | .377489 | 4.295 | -.7328 |
| .0682 | 116 | 4 | 21.1246 | .146922 | .362654 | .373421 | 4.356 | -.6272 |
| .0671 | 118 | 4 | 21.3330 | .147959 | .360050 | .369495 | 4.416 | -.5596 |
| .0660 | 120 | 4 | 21.5245 | .148683 | .357253 | .365704 | 4.477 | -.5092 |
| .0609 | 130 | 4 | 22.4254 | .151096 | .343684 | .348550 | 4.783 | -.3175 |
| .0600 | 132 | 4 | 22.6150 | .151678 | .341359 | .345439 | 4.844 | -.2703 |
| .0587 | 135 | 4 | 22.9336 | .153022 | .338503 | .340952 | 4.936 | -.1659 |
| .0578 | 137 | 4 | 23.2091 | .154803 | .337586 | .338072 | 4.998 | -.0334 |
| .0566 | 140 | 4 | 24.1630 | .165077 | .343958 | .333911 | 5.090 | .7058 |
| .0558 | 142 | 4 | 25.5625 | .182402 | .358772 | .331238 | 5.152 | 1.9618 |
| .0546 | 145 | 5 | 26.3227 | .145907 | .361824 | .370552 | 5.245 | -.6350 |
| .0539 | 147 | 5 | 26.5781 | .147392 | .360381 | .367478 | 5.306 | -.5234 |
| .0528 | 150 | 5 | 26.8866 | .148553 | .357297 | .363023 | 5.399 | -.4309 |
| .0511 | 155 | 5 | 27.3415 | .149627 | .351659 | .355988 | 5.554 | -.3366 |
| .0495 | 160 | 5 | 27.7819 | .150454 | .346192 | .349401 | 5.709 | -.2576 |
| .0480 | 165 | 5 | 28.2565 | .151645 | .341469 | .343221 | 5.864 | -.1450 |
| .0466 | 170 | 5 | 29.0060 | .155989 | .340247 | .337411 | 6.020 | .2417 |
| .0458 | 173 | 5 | 30.8299 | .174316 | .355388 | .334089 | 6.113 | 1.8477 |
| .0453 | 175 | 6 | 31.5768 | .145039 | .359849 | .367740 | 6.175 | -.6924 |
| .0440 | 180 | 6 | 32.2432 | .148407 | .357266 | .361585 | 6.331 | -.3898 |
| .0428 | 185 | 6 | 32.7071 | .149407 | .352637 | .355766 | 6.487 | -.2903 |
| .0417 | 190 | 6 | 33.1419 | .150051 | .347947 | .350259 | 6.643 | -.2202 |
| .0407 | 195 | 6 | 33.5972 | .150871 | .343706 | .345037 | 6.799 | -.1301 |
| .0396 | 200 | 6 | 34.1751 | .152873 | .340899 | .340079 | 6.956 | .0822 |

TABLE A(5)

ESTAR = .41

| LAMBUASTAR | L | ETA | ETASTARTILDA | ETASTAR | ETASTARCALC | ETARES |
|------------|-----|---------|--------------|---------|-------------|--------|
| 5.2984 | 1 | .0308 | .040625 | .040625 | -8.623978 | 6.5792 |
| 3.1791 | 2 | .1666 | .131680 | .131680 | -2.857268 | 3.7826 |
| 1.4450 | 5 | .5249 | .188546 | .188546 | -.283695 | 1.3148 |
| .7569 | 10 | 1.2339 | .232152 | .232152 | .202619 | .1570 |
| .5128 | 15 | 3.1971 | .407467 | .407467 | .302121 | .8266 |
| .4542 | 17 | 3.9178 | .442255 | .442255 | .320307 | 1.0803 |
| .4296 | 18 | 4.1427 | .442362 | .442362 | .327270 | 1.0778 |
| .4076 | 19 | 4.3246 | .438104 | .438104 | .333189 | 1.0356 |
| .3877 | 20 | 4.4812 | .431821 | .431821 | .338264 | .9709 |
| .3117 | 25 | 5.1137 | .396155 | .396155 | .355328 | .5270 |
| .2606 | 30 | 5.6892 | .368487 | .368487 | .364712 | .0583 |
| .2239 | 35 | 6.3282 | .352145 | .352145 | .370419 | .3284 |
| .1962 | 40 | 7.3340 | .357731 | .357731 | .374146 | .3365 |
| .1747 | 45 | 9.1613 | .397752 | .397752 | .376713 | .4846 |
| .1574 | 50 | 10.1411 | .396700 | .396700 | .378556 | .4638 |
| .1314 | 60 | 11.4726 | .374606 | .374606 | .380967 | .1948 |
| .1177 | 67 | 12.7033 | .371774 | .371774 | .382056 | .3513 |
| .1053 | 75 | 14.9872 | .392140 | .392140 | .382949 | .3513 |
| .0987 | 80 | 15.8615 | .389240 | .389240 | .383377 | .2389 |
| .0930 | 85 | 16.5841 | .383173 | .383173 | .383733 | .0242 |
| .0878 | 90 | 17.3407 | .378518 | .378518 | .384031 | .2526 |
| .0832 | 95 | 18.3179 | .378914 | .378914 | .384283 | .2595 |
| .0791 | 100 | 19.6505 | .386256 | .386256 | .384499 | .0894 |
| .0753 | 105 | 20.7827 | .389150 | .389150 | .384685 | .2385 |
| .0719 | 110 | 21.6275 | .386645 | .386645 | .384846 | .1007 |
| .0688 | 115 | 22.4079 | .383254 | .383254 | .384986 | .1013 |
| .0660 | 120 | 23.2723 | .381522 | .381522 | .385110 | .2188 |
| .0633 | 125 | 24.3672 | .383558 | .383558 | .385219 | .1055 |
| .0609 | 130 | 25.5804 | .387227 | .387227 | .385316 | .1262 |
| .0587 | 135 | 26.5816 | .387535 | .387535 | .385402 | .1463 |
| .0566 | 140 | 27.4318 | .385696 | .385696 | .385479 | .0154 |
| .0546 | 145 | 28.2755 | .383897 | .383897 | .385548 | .1216 |
| .0528 | 150 | 29.2319 | .383697 | .383697 | .385611 | .1458 |
| .0511 | 155 | 30.3506 | .385571 | .385571 | .385668 | .0076 |
| .0495 | 160 | 31.4488 | .387077 | .387077 | .385719 | .1104 |
| .0480 | 165 | 32.3951 | .386678 | .386678 | .385766 | .0765 |
| .0466 | 170 | 33.2680 | .385452 | .385452 | .385809 | .0308 |
| .0453 | 175 | 34.1719 | .384645 | .384645 | .385848 | .1068 |
| .0440 | 180 | 35.1841 | .385068 | .385068 | .385884 | .0745 |
| .0428 | 185 | 36.2729 | .386284 | .386284 | .385917 | .0345 |
| .0417 | 190 | 37.2973 | .386768 | .386768 | .385947 | .0791 |
| .0407 | 195 | 38.2261 | .386261 | .386261 | .385976 | .0282 |
| .0396 | 200 | 39.1289 | .385524 | .385524 | .386002 | .0485 |

TABLE A(6)

ESTAR = .45

| LAMBDASTAR | L | ETA | ETASTARTILDA | ETASTAR | ETASTARCALC | ETARES |
|------------|-----|---------|--------------|---------|-------------|--------|
| 5.2984 | 1 | .0311 | .039047 | .039047 | -1.636087 | 1.3326 |
| 3.1791 | 2 | .1866 | .140724 | .140724 | -.301259 | .5860 |
| 2.2708 | 3 | .3383 | .182270 | .182270 | .066499 | .2149 |
| 1.4450 | 5 | .6664 | .228464 | .228464 | .294449 | .1925 |
| 1.0597 | 7 | 1.0719 | .269490 | .269490 | .366154 | .3845 |
| .7569 | 10 | 2.0183 | .362452 | .362452 | .407016 | .2482 |
| .6358 | 12 | 2.8847 | .435149 | .435149 | .419547 | .1034 |
| .5887 | 13 | 3.2709 | .456870 | .456870 | .423832 | .2365 |
| .5128 | 15 | 3.8694 | .470718 | .470718 | .430048 | .3343 |
| .4542 | 17 | 4.3252 | .466035 | .466035 | .434258 | .2949 |
| .4296 | 18 | 4.5278 | .461493 | .461493 | .435870 | .2514 |
| .3877 | 20 | 4.9122 | .451831 | .451831 | .438414 | .1459 |
| .3117 | 25 | 5.8880 | .435390 | .435390 | .442364 | .0943 |
| .2890 | 27 | 6.3241 | .433629 | .433629 | .443376 | .1421 |
| .2606 | 30 | 7.0579 | .436344 | .436344 | .444536 | .1325 |
| .2239 | 35 | 8.4134 | .446884 | .446884 | .445857 | .0193 |
| .1962 | 40 | 9.6616 | .449827 | .449827 | .446720 | .0667 |
| .1747 | 45 | 10.8006 | .447601 | .447601 | .447314 | .0069 |
| .1574 | 50 | 11.9578 | .446493 | .446493 | .447741 | .0334 |
| .1432 | 55 | 13.1738 | .447582 | .447582 | .448057 | .0140 |
| .1314 | 60 | 14.3977 | .448738 | .448738 | .448299 | .0141 |
| .1213 | 65 | 15.5904 | .448819 | .448819 | .448487 | .0115 |
| .1127 | 70 | 16.7706 | .448554 | .448554 | .448637 | .0031 |
| .0987 | 80 | 19.1633 | .448877 | .448877 | .448857 | .0009 |
| .0878 | 90 | 21.5519 | .449045 | .449045 | .449008 | .0018 |
| .0791 | 100 | 23.9369 | .449113 | .449113 | .449116 | .0002 |
| .0528 | 150 | 35.8671 | .449380 | .449380 | .449374 | .0005 |

ESTAR = .60

| LAMBDASTAR | L | ETA | ETASTARTILDA | ETASTAR | ETASTARCALC | ETARES |
|------------|-----|---------|--------------|---------|-------------|--------|
| 5.2984 | 1 | .0274 | .029865 | .029865 | -.352914 | .3516 |
| 3.1791 | 2 | .2486 | .162379 | .162379 | .181462 | .0292 |
| 2.2708 | 3 | .5059 | .236019 | .236019 | .328688 | .1986 |
| 1.4450 | 5 | 1.1629 | .345262 | .345262 | .419944 | .2515 |
| 1.2227 | 6 | 1.5536 | .390321 | .390321 | .437583 | .1881 |
| 1.0597 | 7 | 1.9569 | .426083 | .426083 | .448651 | .1036 |
| .9350 | 8 | 2.3462 | .450737 | .450737 | .456047 | .0276 |
| .8366 | 9 | 2.7079 | .465479 | .465479 | .461233 | .0247 |
| .7569 | 10 | 3.0423 | .473154 | .473154 | .465009 | .0524 |
| .5128 | 15 | 4.5243 | .476658 | .476658 | .474229 | .0231 |
| .3877 | 20 | 5.9914 | .477266 | .477266 | .477579 | .0039 |
| .3117 | 25 | 7.4844 | .479290 | .479290 | .479160 | .0020 |
| .2606 | 30 | 8.9689 | .480202 | .480202 | .480029 | .0032 |
| .1574 | 50 | 14.8859 | .481358 | .481358 | .481312 | .0014 |
| .1053 | 75 | 22.2727 | .481737 | .481737 | .481719 | .0008 |
| .0987 | 80 | 23.7495 | .481774 | .481774 | .481759 | .0007 |
| .0878 | 90 | 26.7028 | .481829 | .481829 | .481820 | .0005 |
| .0791 | 100 | 29.6557 | .481867 | .481867 | .481863 | .0002 |
| .0660 | 120 | 35.5608 | .481914 | .481914 | .481920 | .0004 |
| .0587 | 135 | 39.9887 | .481928 | .481928 | .481947 | .0015 |
| .0528 | 150 | 44.4160 | .481934 | .481934 | .481966 | .0030 |
| .0453 | 175 | 51.8000 | .481989 | .481989 | .481988 | .0001 |
| .0396 | 200 | 59.1806 | .482003 | .482003 | .482002 | .0000 |

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TABLE A(7)