A MODEL OF COMPRESSED MOLECULAR HYDROGEN
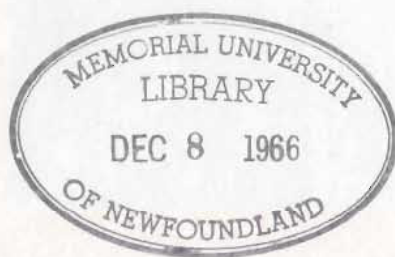
M. F. JONES

A MODEL OF COMPRESSED

MOLECULAR HYDROGEN.

ⓒ M.F. JONES, B.Sc.(Sheffield).

SUBMITTED IN PARTIAL FULFILLMENT OF THE

REQUIREMENTS FOR THE DEGREE OF

MASTER OF SCIENCE

MEMORIAL UNIVERSITY OF NEWFOUNDLAND

MARCH 1966.

ERRATA

page 11, line 3
        for   sectins   read   sections

page 19, line 21
        for ∂V read $\partial(\ln V)$

page 21, line 5
        for   seperated   read   separated

    line 6
        for   distanc)   read   distance)

    line 14
        for   therfore   read   therefore

page 22, line 3
        should read

$$Q = 0.2800.10^{-16}(R^2 - \sum_{\lambda=1}^{2} < 3z_{\lambda}^2 - r_{\lambda}^2 >) \quad cm^2$$

page 23, line 8
        for   for   read   results for

    line 11
        for   its   read   this

    line 13
        for   rotational constant, B_o,
        read   frequency of the $S_o(0)$ spectral line

ABSTRACT

A model of compressed molecular hydrogen is studied in some detail. The model, which had been applied previously to several two and three particle systems, considers the effects of enclosing a single molecule in a rigid spheroidal container, the size of which is related to the pressure of the gas. The resulting Schrodinger wave equation was solved by the variational method. The lack of experimental data precludes any firm conclusion as to the model's adequacy, but it is clear that a model of considerably greater complexity is needed for an adequate treatment.

ACKNOWLEDGEMENTS

TABLE OF CONTENTS

1. INTRODUCTION

In any gaseous system, collisions continually occur and cause instantaneous deformations of the molecules' electronic clouds. The higher the pressure, the greater will be the average deformation. Many of the system's physical properties are determined by the electronic charge distribution, and will thus be pressure-dependant. Thus, the time-independant effects of pressure can be approximated by finding the average charge distribution at various pressures.

A method of doing this was first proposed by Michels, de Boer and Bijl [1]), who considered the effects of enclosing a single hydrogen atom in a rigid spherical container. The instantaneous deformations are thus replaced by a continuous deformation, whilst the exchange effects are completely ignored. The model will possibly be inadequate at low pressures, for here the electronic clouds remain undisturbed for long periods of time; and probably so at high pressures, for here the exchange effects become increasingly important. However, the model gave reasonable results at intermediate pressures.

In their treatment of the hydrogen atom, the usual boundary condition that the electronic wave function should vanish at an infinite distance from the nucleus, was replaced by the condition that it should have a node at a finite distance from it, corresponding to the radius, r_0, of the container, and that it should be strictly zero outside that radius. They developed an approximate solution of the wave equation

which was valid for large r_0. The standard thermodynamic relation

$$P = -\partial E/\partial V$$

$$= -(1/4\pi r_0^2).\partial E/\partial r_0$$

where P is the pressure on the system and V the volume it occupies, then gave the pressure-dependance of the ground state energy, E, whilst Schottky's relation [2]), see also Michels et al [1]),

$$K_t = -E + 3PV$$

where K_t is the total kinetic energy of the electrons and nuclei, gave the pressure-dependance of the internal electronic kinetic energy, K. Schottky's relation enables the total kinetic energy to be determined from isotherm data, and has been tabulated for a variety of gases [3]). This was their comparison with experiment, and they demonstrated that the computed change in the internal electronic kinetic energy of the hydrogen atom is of the same order of magnitude as that which is found for several gases, occurring in bulk.

Sommerfeld and Welker [4]) later gave solutions which were valid for small values of the radius, whilst de Groot and ten Seldam [5]) obtained exact solutions for the ground state energy, the ground state being a 1s state. These latter also gave approximate solutions for the 2s and 2p states.

Cottrell [6]) considered the analagous problem for the hydrogen-molecular ion; again the only comparison with experiment being the variation of the internal electronic kinetic energy. In this instance,

the wave equation was solved using the variational technique, the chosen wave function being

$$\psi = e^{-\delta\xi}(1 + \eta^2/2)(\xi_0 - \xi)$$

where δ is the variational parameter and ξ, η are the usual prolate spheroidal coordinates with

$$1 \leq \xi \leq \xi_0 \quad , \quad -1 \leq \eta \leq +1$$

and ξ_0 specifies the size of the spheroidal container.

ten Seldam and de Groot [7] applied the treatment to the helium atom; the variational wave function being chosen as

$$\psi = e^{-S/2}(C_0 + C_1 U + C_2 T^2)(1 - (S - T)/2R)(1 - (S + T)/2R)$$

where $S = k(r_2 + r_1)$

               $T = k(r_2 - r_1)$

               $U = kr_{12}$

and $R = kr_0$

with r_1 being the distance of electron i from the nucleus, r_{12} the distance between the two electrons, k, C_0, C_1, C_2 the variational parameters and r_0 the radius of the container.

The present work has been to treat, in a similar manner, the simplest molecular system, namely the hydrogen molecule. Difficulties were encountered in the evaluation of the exchange integrals (with finite upper limits, rather than the usual infinite ones). This, in large measure, determined the the choice of variational wave function.

2. MATHEMATICAL METHOD

The time-independant Schrodinger wave equation may be written as

$$H\psi = E\psi$$

where H is the Hamiltonian of the system and ψ its electronic wave function. If atomic units are used, that is 1 au of length = 1 Bohr radius = $0.52917.10^{-8}$ cms, and 1 au of energy = 2 Rydbergs = 27.210 ev, then the Hamiltonian of the hydrogen molecule is

$$H = -(\Delta_1^2 + \Delta_2^2)/2 + V$$

where V is the potential energy of the molecule and

$$-V = 1/r_{1a} + 1/r_{2a} + 1/r_{1b} + 1/r_{2b} - 1/r_{12} - 1/R$$

with the coordinate system shown in Fig. 1.
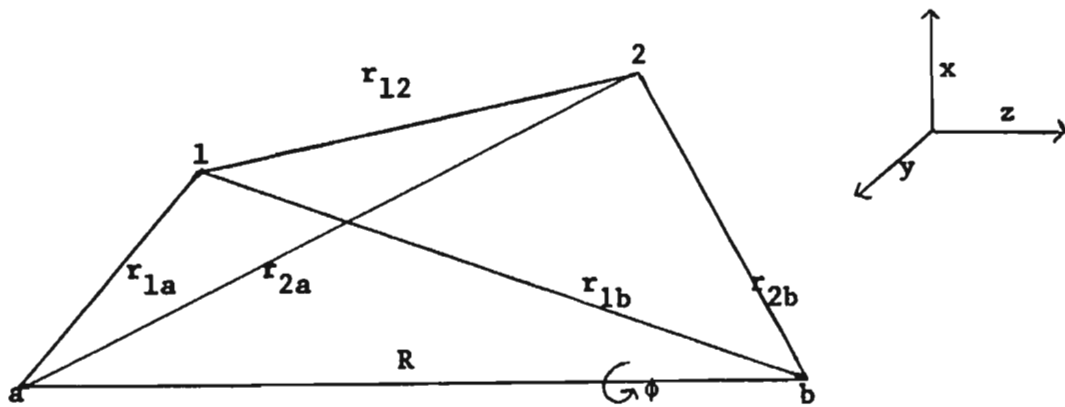
FIG. 1

If we now define prolate spheroidal coordinates as

$$\xi_1 = (r_{1a} + r_{1b})/R$$

$$\eta_1 = (r_{1a} - r_{1b})/R$$

$$\phi_i = \tan^{-1}(y_i/x_i)$$

with $i = 1,2$ and where, for the free molecule

$$1 \leq \xi_1, \xi_2 \leq \infty$$

$$-1 \leq \eta_1, \eta_2 \leq +1$$

$$0 \leq \phi_1, \phi_2 \leq 2\pi$$

then the Laplacian becomes

$$\Delta_i^2 = \frac{4}{R^2(\xi_i^2 - \eta_i^2)} \left| \frac{\partial}{\partial \xi_i} (\xi_i^2 - 1) \frac{\partial \psi}{\partial \xi_i} + \frac{\partial}{\partial \eta_i} (1 - \eta_i^2) \frac{\partial \psi}{\partial \eta_i} \right.$$

$$\left. + \frac{\eta_i^2 - \xi_i^2}{(\xi_i^2 - 1)(\eta_i^2 - 1)} \frac{\partial^2 \psi}{\partial \phi_i^2} \right|, \quad i = 1,2$$

whilst the potential energy is given by

$$V = -\frac{4}{R} \left| \frac{\xi_1}{\xi_1^2 - \eta_1^2} + \frac{\xi_2}{\xi_2^2 - \eta_2^2} \right| + \frac{1}{R} + \frac{1}{r_{12}}$$

where

$$(2/R)^2 r_{12}^2 = \xi_1^2 + \xi_2^2 + \eta_1^2 + \eta_2^2 - 2 - 2\xi_1 \xi_2 \eta_1 \eta_2$$

$$- 2\cos(\phi_1 - \phi_2)((\xi_1^2 - 1)(\xi_2^2 - 1)(\eta_1^2 - 1)(\eta_2^2 - 1))^{\frac{1}{2}}$$

2.1

For our purposes, the electronic wave function of compressed hydrogen is expressed as a linear combination of

$$\psi_1 = \psi_a(1) + \psi_b(2)$$

and $\quad \psi_2 = \psi_a(2) + \psi_b(1)$

in the form

$$\Psi = \psi_1 \pm \psi_2$$

with the upper sign for the singlet state, the lower for the triplet, and where

$$\psi_a(i) = e^{-\alpha\xi_i} e^{-\beta\eta_i} (1 - \xi_i/\xi_0)$$

$$i = 1,2$$

$$\psi_b(i) = e^{-\alpha\xi_i} e^{+\beta\eta_i} (1 - \xi_i/\xi_o)$$

where α, β are the variational parameters and

$$1 \leq \xi_1, \xi_2 \leq \xi_0$$

with ξ_0 specifying the container size.

Thus for the singlet state

$$\psi_s = e^{-\alpha(\xi_1 + \xi_2)} (\cosh\beta(\eta_1 - \eta_2))(1 - \xi_1/\xi_0)(1 - \xi_2/\xi_0)$$

whilst for the triplet state

$$\psi_t = e^{-\alpha(\xi_1 + \xi_2)} (\sinh\beta(\eta_1 - \eta_2))(1 - \xi_1/\xi_0)(1 - \xi_2/\xi_0)$$

These wave functions reduce, when $\xi_0 = \infty$, to those treated by Inui [8] and by Norsdieck [9]. Using the singlet wave function, Inui found the binding energy of molecular hydrogen to be 4.058 ev, and the equilibrium internuclear distance to be 1.44 au; the present work gives the internuclear distance as 1.42 au and the binding energy as 4.061 ev, the difference arising from the avoidance of interpolation techniques. It will be recalled that the experimental binding energy is 4.746 ev with an internuclear distance of 1.40008 au. Thus even if the model is

essentially correct at low pressures, the results obtained here will
not tally with experiment. This did not apply to previous studies of
this type, for in these either the wave equation was solved exactly or
the variational wave function was very good at zero pressure.

2.2

If we now let

$$H_1 = \int \psi_a(1)\psi_b(2)\, H\, \psi_a(1)\psi_b(2)\, d\tau$$

$$H_{11} = \int \psi_a(1)\psi_b(2)\, H\, \psi_a(2)\psi_b(1)\, d\tau$$

$$S_1 = \int \psi_a^2(1)\psi_b^2(1)\, d\tau$$

and $$S_{11} = \int \psi_a(1)\psi_a(2)\psi_b(1)\psi_b(2)\, d\tau$$

where $$d\tau = (R/2)^6 (\xi_1^2 - \eta_1^2)(\xi_1^2 - \eta_1^2)\, d\xi_1 d\xi_2 d\bar{\eta}_1 d\eta_2 d\phi_1 d\phi_2$$

it follows immediately from the form of the chosen wave function that
the ground state energy of the molecule is given by

$$E = (H_1 \pm H_{11})/(S_1 \pm S_{11})$$

the upper signs holding for the singlet state, the lower for the triplet.

After some straight-forward, but lengthy, calculations, we arrive
at the following

$$H_1 = (\pi R^3/4)^2 (4AB/R^2 + (B^2 - CB + D)/R)$$

$$H_{11} = (\pi R^3/4)^2 (4JK/R^2 + (K^2 - LK + M)/R)$$

$$S_1 = (\pi R^3/4)^2 B^2$$

and $$S_{11} = (\pi R^3/4)^2 K^2$$

in the above formulae we have

$$J = 2(U_0(2\alpha,\xi_0) - U_1(2\alpha,\xi_0)) - (2\beta)^2 V_0(2\alpha,\xi_0)/3$$

$$A = B_0(2\beta)(U_0(2\alpha,\xi_0) - U_1(2\alpha,\xi_0)) - \beta B_1(2\beta)V_0(2\alpha,\xi_0)$$

$$K = 2(V_2(2\alpha,\xi_0) - V_0(2\alpha,\xi_0)/3)$$

$$B = B_0(2\beta)V_2(2\alpha,\xi_0) - B_2(2\beta)V_0(2\alpha,\xi_0)$$

$$L = 16V_1(2\alpha,\xi_0)$$

$$C = 8B_0(2\beta)V_1(2\alpha,\xi_0)$$

$$M = 8(X_0(2,2,2\alpha,\xi_0) - 2X_0(0,2,2\alpha,\xi_0)/3$$
$$+ X_0(0,0,2\alpha,\xi_0)/9 + 4X_2(0,0,2\alpha,\xi_0)/45)$$

and
$$D = 2\sum_{\tau=0}^{\infty} (-1)^\tau (2\tau + 1)(X_\tau(2,2,2\alpha,\xi_0)G_\tau^2(0,2\beta)$$
$$- 2X_\tau(0,2,2\alpha,\xi_0)G_\tau(0,2\beta)G_\tau(2,2\beta) + X_\tau(0,0,2\alpha,\xi_0)G_\tau^2(2,2\beta))$$

We have the further formulae

$$U_n(2\alpha,\xi_0) = ((\alpha^2 + 2\alpha/\xi_0)A_n(2\alpha,\xi_0) - (\alpha^2 + 4\alpha/\xi_0)A_{n+2}(2\alpha,\xi_0)$$
$$+ (2\alpha - (\alpha^2 + 2)/\xi_0)A_{n+1}(2\alpha,\xi_0) + \alpha^2 A_{n+3}(2\alpha,\xi_0)/\xi_0)/\xi_0^n$$

and
$$V_n(2\alpha,\xi_0) = A_n(2\alpha,\xi_0) - 2A_{n+1}(2\alpha,\xi_0)/\xi_0 + A_{n+2}(2\alpha,\xi_0)/\xi_0^2$$

where
$$A_n(\alpha,\xi_0) = \int_1^{\xi_0} e^{-\alpha x} x^n \, dx$$

$$B_n(\beta) = \int_{-1}^{1} e^{-\beta x} x^n \, dx$$

$$G_\tau(n,\beta) = \int_{-1}^{1} e^{-\alpha x} x^n P_\tau(x) \, dx$$

and
$$X_\tau(m,n,\alpha,\xi_0) =$$

$$\int_1^{\xi_0}\int_1^{\xi_0} e^{-\alpha(\xi_1 + \xi_2)}(1 - \xi_1/\xi_0)^2(1 - \xi_2/\xi_0)^2\xi_1^n\xi_2^m \, Q_\tau\left|\begin{matrix}\xi_2\\\xi_1\end{matrix}\right| P_\tau\left|\begin{matrix}\xi_1\\\xi_2\end{matrix}\right| d\xi_1 d\xi_2$$

These X_τ functions may be expressed as linear combinations of

$$W_\tau(m,n,\alpha,\xi_0) = \int_1^{\xi_0}\int_1^{\xi_0} e^{-\alpha(\xi_1 + \xi_2)}\xi_1^n\xi_2^m Q_\tau\left|\begin{matrix}\xi_2\\\xi_1\end{matrix}\right| P_\tau\left|\begin{matrix}\xi_1\\\xi_2\end{matrix}\right| d\xi_1 d\xi_2$$

$$= W_\tau(n,m,\alpha,\xi_0)$$

the upper variables in Q_τ and P_τ being used when $\xi_1 > \xi_2$, the lower when $\xi_2 > \xi_1$. The P_τ and Q_τ are the Legendre functions of the 1st and 2nd kind respectively, and are defined in Abramowitz and Stegun [10].

In the derivation of the above formulae for M and for D, the standard Neumann Expansion of $1/r_{12}$ was used, the only terms of which that are non-vanishing on integration over the angles being

$$(2/R) \sum_{\tau=0}^{\infty} (2\tau + 1) P_\tau \left|\begin{matrix} \xi_1 \\ \xi_2 \end{matrix}\right| Q_\tau \left|\begin{matrix} \xi_2 \\ \xi_1 \end{matrix}\right| P_\tau(\eta_1) P_\tau(\eta_2)$$

with our previous notation.

The ground state energy of the singlet state is then given by

$$E = 2a(\alpha,\beta,\xi_0)/R^2 - b(\alpha,\beta,\xi_0)/R$$

where $\quad a(\alpha,\beta,\xi_0) = (AB + JK)/(B^2 + K^2)$

and $\quad b(\alpha,\beta,\xi_0) = -1 + (BC + KL - D - M)/(B^2 + K^2)$.

Thus, if these functions are evaluated for a given α,β pair, then for that pair the internuclear distance for which the energy is a minimum is given by

$$R = 4a(\alpha,\beta,\xi_0)/b(\alpha,\beta,\xi_0)$$

whilst the corresponding minimum is

$$E = -b^2(\alpha,\beta,\xi_0)/8a(\alpha,\beta,\xi_0).$$

The energy was minimised for eleven selected values of ξ_0 to eight significant figures, with an accuracy of ± 0.00025 in α and β. The results obtained by taking the first four and five terms in the

Neumann expansion are given in Tables 1 and 2 respectively; all tables are given in Appendix 1. It will be noted that only in the case of $\xi_0 = 4$, is the difference between the energy values greater than 3 units in the 5th decimal place.

2.3

The electronic charge distribution determines many of the molecules physical properties and it was thought of interest to find the pressure dependance of some measures of this distribution. In general, these measures are expressible as linear combinations of terms as $\xi^m \eta^n$ and it follows straight-forwardly that

$$< \xi^m \eta^n > = (H(m,n) \pm F(m,n))/(B^2 \pm K^2)$$

with the upper signs being used for the singlet state, the lower for the triplet.

In the above, if m is even

$$H(m,n) = B.(V_{n+2}(2\alpha,\xi_0)B_m(2\beta) - V_n(2\alpha,\xi_0)B_{m+2}(2\beta))$$

and

$$F(m,n) = 2K.(V_{n+2}(2\alpha,\xi_0)/(m + 1) - V_n(2\alpha,\xi_0)/(m + 3))$$

whilst if m is odd

$$H(m,n) = F(m,n) = 0.$$

3. COMPUTATIONAL PROCEDURES

Extensive tables exist for the functions to be considered in sectins 3.1 and 3.2 and for all of the other necessary functions when $\xi_0 = \infty$. However, because of the complexity of the necessary interpolation formulae and because of the relative smallness of the computer used in this investigation (an IBM 1620 Model 1 with 40K storage), it was decided to make the energy evaluation completely independant of existing tables, using them, where possible, as checks of the programmes' accuracy; except where stated to the contrary, these programmes were written to use 8 figure arithmetic. The general methods of Zener and Guillemin [11]), Bartlett [12]), Rosen [13]), Kotani, Amemiya, Ishiguro and Kimura [14]) and of Rudenberg [15]) were followed in the evaluation of the integrals, whilst the notation given in a review article by Dalgarno [16]) was adhered to.

3.1 Ei(-x)

The exponential integral is defined as

$$Ei(-x) = \int_x^\infty (e^{-y}/y) \, dy.$$

When the exponential is expanded under the integral sign and the resulting series integrated term by term, the following series expansion is found

$$Ei(-x) = C + \ln(x) + \sum_{n=0}^\infty (-x)^n/(n.n!)$$

where C is Euler's constant $= 0.57721...$

For $x \leq 2$, the first fifteen terms of this series were used to

evaluate the function, whilst for the rest of the range a 15-point
Laguerre-Gaussian quadrature was used (only the first 10 points
contributing to the integral). The values given by this scheme were
checked against the extensive tabulations in Abramowitz et al [10]. At
no point did the values differ in the 7th figure, whilst in most cases
the values agreed to within 2 or 3 units in the 8th.

3.2 $B_n(\beta)$

$$B_n(\beta) = \int_{-1}^{1} e^{-\beta x} x^n \, dx$$

When the above is integrated by parts, the following recursion
formula is obtained

$$B_n(\beta) = ((-1)^n e^{\beta} - e^{-\beta} + nB_{n-1}(\beta))/\beta.$$

This was used in the backward direction, and was initiated by setting
$B_{31}(\beta)$ to zero, only values $0 \le n \le 10$ being required. Spot checks in
the tables of Miller, Gerhauser and Matsen [17] showed discrepancies
of 3 or 4 units in the 8th figure.

3.3 $G_{\tau}(n,\beta)$

$$G_{\tau}(n,\beta) = \int_{-1}^{1} e^{-\beta x} x^n P_{\tau}(x) \, dx$$

where $P_{\tau}(x)$ is the Legendre polynomial. By making use of the well known
recursion formula for these polynomials

$$nP_n(x) = (2n + 1)xP_{n-1}(x) - (n - 1)P_{n-2}(x) \qquad n \ge 2,$$

these $G_{\tau}(n,\beta)$ functions are expressible as linear combinations of the
$B_n(\beta)$ functions discussed in section 3.2, the accuracy of evaluation
being dependant only on the accuracy of those latter functions.

3.4 $A_n(\alpha, \xi_0)$

$$A_n(\alpha, \xi_0) = \int_1^{\xi_0} e^{-\alpha x} x^n \, dx$$

$$= A_n(\alpha) - \xi_0^{n+1} A_n(\alpha \xi_0)$$

where $A_n(\alpha) = A_n(\alpha, \infty)$

and $A_n(\alpha) = (e^{-\alpha} + n A_{n-1}(\alpha))/\alpha$

which recursion formula is obtained on integrating by parts.

For $\xi_0 \geq 25$, the recursion formula gave sufficient accuracy, whilst for values less than this, a 24-point Legendre-Gaussian quadrature was used. It is believed that at least 7 figure accuracy was obtained for the entire range of ξ_0 and for $0 \leq n \leq 15$. This conclusion follows from spot checks in the tables of Miller et al [17], and from the use of higher order gaussian quadratures.

3.5 $W_\tau(m,n,\alpha,\xi_0)$

This is the function introduced in section 2.2 in the expansions of the X_τ functions, it will be recalled that,

$$W_\tau(m,n,\alpha,\xi_0) = \int_1^{\xi_0}\int_1^{\xi_0} e^{-\alpha(\xi_1 + \xi_2)} \xi_1^m \xi_2^n \, Q_\tau \begin{vmatrix} \xi_2 \\ \xi_1 \end{vmatrix} P_\tau \begin{vmatrix} \xi_1 \\ \xi_2 \end{vmatrix} \, d\xi_1 d\xi_2$$

$$= W_\tau(n,m,\alpha,\xi_0)$$

the upper variables in Q_τ and P_τ being used when $\xi_2 > \xi_1$, the lower when $\xi_1 > \xi_2$.

The recursion formulae given by Rudenberg [15], Kotani et al [14] and by James [18] are easily generalised to include the finite upper

limit, but are found to be quite useless for computational purposes because of the rapid loss of significant figures. A simple crossed gaussian quadrature scheme was tried, but was found to be prohibitively long in computation time.

Such direct evaluations of the W_τ functions were thus discarded, use being made of the following auxiliary functions: $Q_\tau(x)$, $F_\tau(m,\alpha,\xi_0)$, $G_m(\alpha,\xi_0)$ and $SS_\tau(k,m,\alpha,\xi_0)$, to be defined below.

3.5.1 $Q_\tau(x)$

This is the Legendre function of the 2nd kind as defined in Abramowitz et al [10]); it will be recalled that this function has a logarithmic singularity at $x = 1$. For $x > 2.5$, the hypergeometric series expansion given in Abramowitz et al [10]) gave 7 to 8 figure accuracy, but was quite useless for arguments less than this. The function values are needed in the gaussian quadratures to be mentioned in sections 3.5.2 b) and d), and for each ξ_0 is independant of both α and β. Therefore, a separate programme was written, in 28 figure arithmetic, which used the explicit expressions for Q_1 and Q_3, the output of which was rounded to 8 significant figures. We have

$$Q_1(x) = xQ_0(x) - 1$$
$$Q_3(x) = (5x^3 - 3x)Q_0(x)/2 - 5x^2 + 2/3$$

where $Q_0(x) = \ln((1 + x)/(x - 1))/2$

3.5.2 $F_\tau(m\ \alpha\ \xi_0)$

$$F_\tau(m,\alpha,\xi_0) = \int_1^{\xi_0} e^{-\alpha x} x^m Q_\tau(x)\ dx$$

The following recursion formula follows immediately from that of the Q_τ functions, if $\tau \geq 2$

$$\tau F_\tau(m,\alpha,\xi_0) = (2\tau + 1)F_{\tau-1}(m + 1,\alpha,\xi_0) - (\tau - 1)F_{\tau-2}(m,\alpha,\xi_0)$$

and was used extensively. Particular τ values are now examined separately:

a) $\tau = 0$

If, generalising Rudenberg [15]), we define

$$G_m(\alpha,\xi_0) = (-1)^m (d^m/d\alpha^m) (\alpha F_0(0,\alpha,\xi_0)),$$

then
$$G_0(\alpha,\xi_0) = e^{-\alpha}(C + \ln(2\alpha) - Ei(-\alpha(\xi_0 - 1)) - 2Q_0(\xi_0)e^{-\alpha\xi_0}$$
$$- e^{2\alpha}(Ei(-2\alpha) - Ei(-\alpha(\xi_0 + 1)))$$

$$G_1(\alpha,\xi_0) = e^{-\alpha}(C + \ln(2\alpha) - Ei(-\alpha(\xi_0 - 1)) - 2\xi_0 Q_0(\xi_0)e^{-\alpha\xi_0}$$
$$+ e^{2\alpha}(Ei(-2\alpha) - Ei(-\alpha(\xi_0 + 1)))$$

and
$$G_m(\alpha,\xi_0) = G_{m-2}(\alpha,\xi_0) - A_{m-2}(\alpha,\xi_0) - \xi_0^m(\xi_0^2 - 1)Q_0(\xi_0)e^{-\alpha\xi_0} , m > 2$$

where C is Euler's constant $= 0.57721...$ The $F_0(m,\alpha,\xi_0)$ are now given by

$$F_0(m,\alpha,\xi_0) = (mF_0(m - 1,\alpha,\xi_0) + G_m(\alpha,\xi_0))/\alpha$$

and this last expression was used throughout.

b) $\tau = 1$

The recursion formula

$$F_1(m,\alpha,\xi_0) = F_1(m + 1,\alpha,\xi_0) - A_m(\alpha,\xi_0)$$

loses accuracy quite rapidly for $m > 4$. Beyond this value, the integral was evaluated by splitting the interval into three parts, $1 \to 1.01$, $1.01 \to 1.40$ and $1.40 \to \xi_0$ and using a 48-point Legendre-Gaussian

quadrature for each part. Spot checks in the tables of Kotani et al [14] showed, for $\xi_0 = \infty$, discrepancies of 3 or 4 units in the 8th figure.

c) $\tau = 2$

The recursion formulae

$$F_2(1,\alpha,\xi_0) = (3F_1(2,\alpha,\xi_0) - F_0(1,\alpha,\xi_0))/2$$

and

$$F_2(m,\alpha,\xi_0) = (3F_3(m - 1,\alpha,\xi_0) + 2F_1(m - 1,\alpha,\xi_0))/5 \quad, m > 1$$

yielded sufficient accuracy.

d) $\tau = 3$

For all m, these integrals were evaluated using the same quadrature scheme as that outlined in section 3.5.2 b).

e) $\tau = 4$

For all m, the recursion formula

$$F_4(m,\alpha,\xi_0) = (7F_3(m + 1,\alpha,\xi_0) - 3F_2(m,\alpha,\xi_0))/4$$

gave at least 5 figure accuracy.

3.5.3 $SS_\tau(k,m,n,\alpha,\xi_0)$

Let us define

$$SS_\tau(k,m,n,\alpha,\xi_0) = S_\tau(m,n + k,\alpha,\xi_0) + S_\tau(m + k,n,\alpha,\xi_0)$$

where

$$S_\tau(m,n,\alpha,\xi_0) = \int_1^{\xi_0} e^{-\alpha x} x^m Q_\tau(x) \left| \int_1^x e^{-\alpha y} y^n \, dy \right| dx$$

and

$$S_\tau(m,n,\alpha,\xi_0) = (nS_\tau(m,n - 1,\alpha,\xi_0) - F_\tau(m + n,2\alpha,\xi_0)$$

$$- e^{-\alpha}F_\tau(m,\alpha,\xi_0))/\alpha.$$

The S_τ function is a generalisation of Kotani's S function [14],
and the above formulae were used in its evaluation.

We are now in a position to reconsider the the W_τ functions. It
is immediately obvious that

$$W_\tau(m,n,\alpha,\xi_0) = \int_1^{\xi_0} dx \ e^{-\alpha x} \ x^m \ Q_\tau(x) \int_1^x e^{-\alpha y} \ y^n \ P_\tau(y) \ dy$$

$$+ \int_1^{\xi_0} dx \ e^{-\alpha x} \ x^n \ Q_\tau(x) \int_1^x e^{-\alpha y} \ y^m \ P_\tau(y) \ dy$$

and if the explicit expressions for the Legendre polynomial are
substituted into this last expression we obtain

$$W_\tau(m,n,\alpha,\xi_0) = \sum_{\nu=0}^k C_{\tau,\tau-2\nu} \ SS_{\tau-2\nu}(m,n,\alpha,\xi_0)$$

where $\quad k = \tau/2 \qquad \tau$ even

$$= (\tau - 1)/2 \quad \tau \text{ odd}$$

with the $C_{\tau,\nu}$ defined by

$$P_\tau(x) = \sum_{\nu=0}^\tau C_{\tau,\nu} \ x^\nu$$

This expansion of the W_τ function was used to evaluate it, but
before examining the accuracy obtained, let us consider an alternative
scheme for the evaluation of the SS_τ function. We define

$$TT_\tau(k,m,n,\alpha,\xi_0) = A_{m+k}(\alpha)F_\tau(n,\alpha,\xi_0) - T_\tau(m + k,\alpha,\xi_0)$$

$$+ A_{n+k}(\alpha)F_\tau(m,\alpha,\xi_0) - T_\tau(n + k,\alpha,\xi_0)$$

where $\quad T_\tau(m,n,\alpha,\xi_0) = (m!/\alpha^{m+1}) \sum_{\nu=0}^m \alpha^\nu \ F_\tau(n + \nu,2\alpha,\xi_0)/\nu!$

and $\quad T_\tau(m,n,\alpha,\xi_0) = (mT_\tau(m - 1,n,\alpha,\xi_0) + F_\tau(m + n,2\alpha,\xi_0))/\alpha.$

This T_τ function is a generalisation of Rosen's T function [13], and

if we now observe that

$$\int_1^x e^{-\alpha y} y^n \, dy = A_n(\alpha) - x^{n+1} A_n(\alpha x)$$

where $\quad A_n(x) = e^{-x} n!/x^{n+1} \sum_{\nu=0}^{n} x^\nu/\nu!$

it is apparent that

$$TT_\tau(k,m,n,\alpha,\xi_0) = SS_\tau(k,m,n,\alpha,\xi_0)$$

and that the two functions are formally identical, differing only in the computational procedures.

Of the two schemes, that using the SS_τ function is more accurate when ξ_0 is finite, the two being virtually identical when ξ_0 is infinite. For this value of ξ_0, spot checks in the tables of Miller et al [17] indicate that : for $\tau = 0$, 7-8 figure accuracy is obtained; for $\tau = 1$, 6-7 figures; for $\tau = 2$, 4-6 figures; for $\tau = 3$, 4-6 figures and for $\tau = 4$, 2-3 figures. For other values of ξ_0, checks using the recursion formula developed in Appendix 2 indicate that the accuracy is at least as good as this for ξ_0 greater than about 4.

4. RESULTS

Using four terms in the Neumann expansion of $1/r_{12}$, the ground state energy was minimised (with an accuracy of ± 0.00025 in α and β, the variational parameters) for 11 values of ξ_0, and the results are given in Table 1. The energy values are certainly accurate to 6 significant figures and the internuclear distances to 5. For comparison purposes, the results obtained from the five term Neumann expansion are given in Table 2; this fifth term could not be evaluated at all accurately. It will be observed that only in the case of $\xi_0 = 4$ is the difference between the two energies greater than 3 units in the 5th decimal place.

The gaseous pressure could now be found using graphical differentiation for

$$P = - \partial E/\partial V,$$

where E is the energy of the molecule and V the volume it occupies. However, the graph of E vs V could not be used for this purpose, for the changes in slope are truly enormous. The slope variations in the graph of $-\ln(E - E_0)$ vs $\ln(V)$, where E_0 is the energy at zero pressure, are considerably less, although still of the order 100. The pressure is now given by

$$P = ((E - E_0)/V).\partial(E - E_0)/\partial V$$

and the pressure variation of the internal kinetic energy of the electrons is determined using Schottky's relation [2]. The values obtained are given in Table 3, whilst Fig 2 gives the information in graphical form;

FIG 2

PRESSURE VARIATION OF THE INTERNAL ELECTRONIC KINETIC ENERGY, K.

$\ln(1 + \Delta K)$

ΔK in

kcal/mole

---H_2 (theory)

---H_2 150°C (expt.)

---H_2 150°C (expt.)

$\ln(1 + P)$

P in atmos.
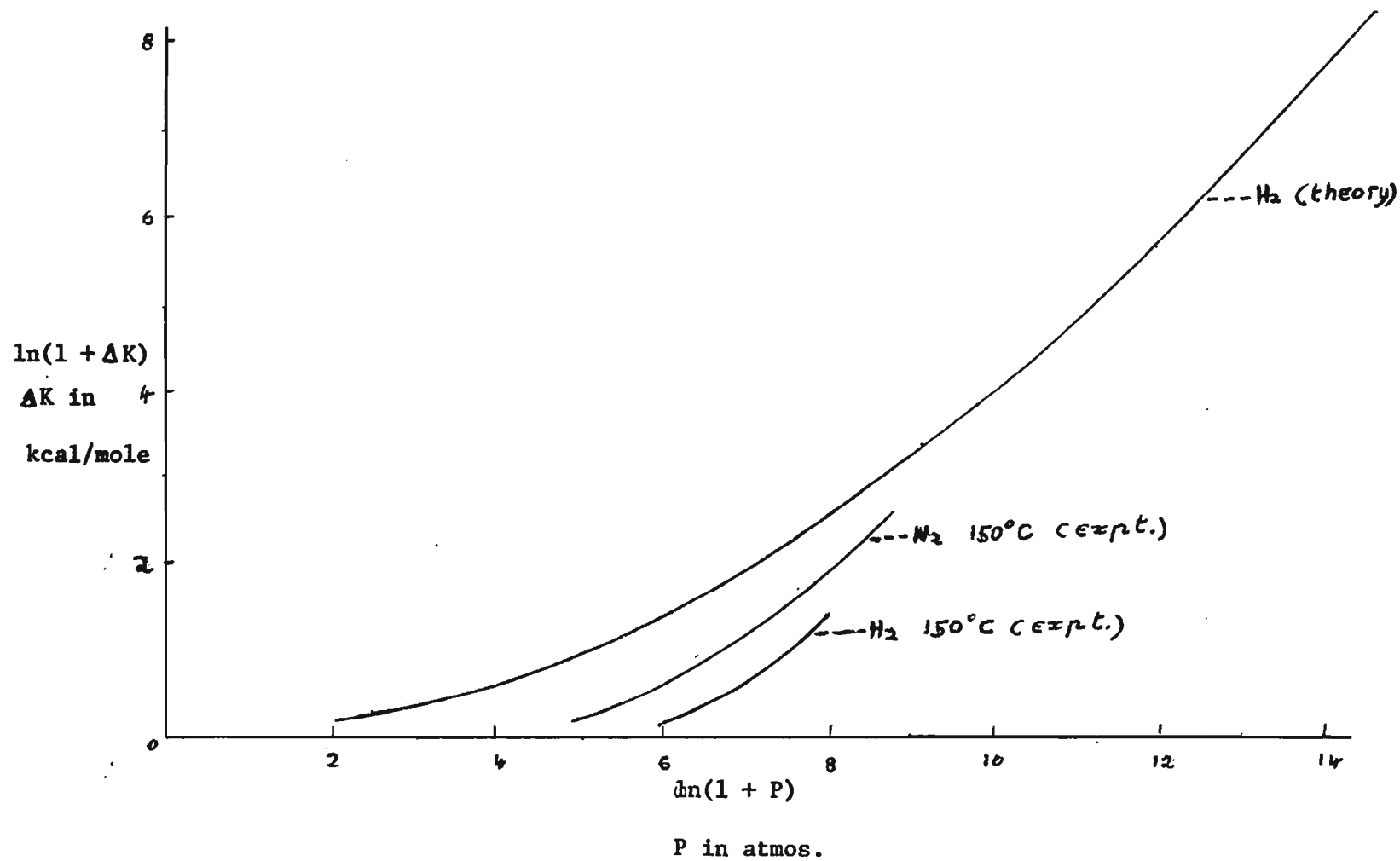
the scales in Fig 2 are pseudo-logarithmic, that is they are linear for small values of the argument and logarithmic for large.

The usual definition of the binding energy of molecular hydrogen (viz: the energy differential between the isolated molecule and the combined energies of two hydrogen atoms seperated by an infinite distanc) is surely inapplicable when the gas is under pressure, for this would immediately imply that the molecule would become less stable as the pressure is increased. It would seem more reasonable to redefine the binding energy as the energy differential between the molecule and the combined energies of its constituents, all particles being under the same conditions. This definition obviously includes the more usual one, but is immediately applicable to high pressure situations. Using the results in [1], [4] and [5] enables the pressure dependance of the ground state energy of atomic hydrogen to be determined and therfore, assuming the new definition, the binding energy of molecular hydrogen. The results of such a procedure are given in Table 4, which also gives the pressure dependance of the internuclear distance; it can be seen that both of these quantities increase with pressure.

Of the several electronic expectation operators investigated, only two are directly related to experiment. The Larmor term in the molar diamagnetic susceptibility is given by Van Vleck as [19]

$$\chi_{\ell} = (Nr_0 a_0^2 \sum_{\lambda=1}^{2} < r_{\lambda}^2 >)/6$$

$$= 1.5847.10^{-6} < r_1^2 > \quad \text{cgs units}$$

where N is Avogadros number, $r_0 = e^2/mc^2$ is the classical electron radius and $a_0 = h^2/4\pi^2 me^2$ is the Bohr radius for infinite nuclear mass.

The molecular quadrupole moment is given by

$$Q = (R^2 - \sum_{\lambda=1}^{2} < 3z_\lambda^2 - r_\lambda^2 >)$$

$$= 0.2800.10^{-16} < 3z_\lambda^2 - r_\lambda^2 > \text{ cm}^2$$

with the first term representing the contribution of the nuclei, see
for example Gordy, Smith and Trambarulo [20]). The pressure variation of
these operators is given in Table 5.

The pressure variation of various other operators are given in
Table 6 for the singlet state, and in Table 7 for the triplet state.
Of these, $< 1/r_{12} >$ is the total electron repulsion energy, whilst the
others give some idea of the electronic charge distribution, for example,
$< \xi >$ gives an indication of the size of the electron cloud.

5. CONCLUSION

Perhaps the most surprising feature of this investigation is the persistent increase of the internuclear distance with pressure. This would seem to imply that the molecule tends to dissociate at high pressures. However, despite this increase, the model does predict an increase of the binding energy, see Table 4. This increase in the internuclear distance is also apparent when one examines Cottrell's [6] for the hydrogen-molecular ion, these are reproduced in Table 8. Unfortunately that author makes no mention of this. The phenomenon appears, therefore, to be characteristic of the general model, and not simply of its particular application.

May, Degen, Stryland and Welsh [21] have studied the Raman spectrum of hydrogen at high pressures, and find that the rotational constant, B_0, increases from 354.38 cm^{-1} at 1 atmosphere pressure to 354.82 cm^{-1} at 1938 atmospheres. This gives a decrease of 0.01% in the internuclear distance, the rotational constant varies inversely as the square of the internuclear distance. The present calculations give an increase of 1.6%.

Much of the following discussion has been derived from the standard reference work by Hirschfelder, Curtiss and Bird [22]. Hellmann [23] and Feynman [24] have proved that the forces acting on the nuclei in any molecular configuration are just those which are to be expected on the basis of classical electrostatics. Certainly the spin and exchange effects play an important role in determining the distribution of charge, but once the distribution is determined, the forces on the nuclei may be found by purely classical means. Berlin [25] has given the following visualisation of the Hellmann-Feynman theorem: on referring to Fig 3,

a)   b)
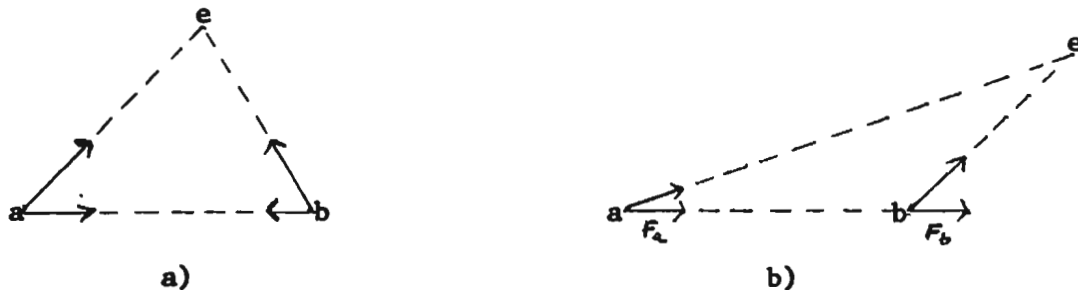
FIG. 3

which shows the forces exerted on nuclei a and b by that part of the electron cloud e, we see that condition a) always tends to bind the nuclei together, whilst condition b) may or may not do so, depending on the relative magnitudes of F_a and F_b; if these two forces are equated, the boundary surfaces between the binding and non-binding regions may be found by a straight-forward application of Coulomb's law.

Now, under increasing pressures, the electron density must certainly increase in the region of the nuclei, and indeed, in Table 6, we see that the size, $< \xi >$, of the electronic cloud shows a persistent decrease. However, this decrease could occur in a variety of ways: if the electron density increases uniformly in the binding and non-binding regions, the internuclear distance would remain constant; if the density increases more in the binding region, the internuclear distance would decrease; and if the density increases more in the non-binding region, the internuclear distance would increase. There are no a priori reasons for rejecting this last alternative.

Thus, the present calculations predict a major regrouping of charge

in the non-binding region, which must lead to an increase in the average inter-electronic distance; this is seen in Table 6 in the decreasing values of $< 1/r_{12} >$. The numerical values of $< z^2 >$, $< r_a >$ and $<r^2 > = < x^2 + y^2 >$ also decrease up to pressures of about 10,000 atmospheres, after which they increase; this behaviour is not really surprising, for initially the boundary condition imposed on the system would lead to a simple contraction of the electron cloud and finally to an elongation of the cloud along the z-axis under the influence of the increasing charge density in the non-binding region. The increase in $< \eta^2 >$ would be consistent with this interpretation for $\eta = (r_a - r_b)/R$. The same general trends in the operators are seen for the triplet state, see Table 7.

It is difficult to assess the physical significance of the model because of the lack of experimental data. Indeed, the two comparisons with experiment given are both suspect. In Schottky's formula

$$K_t = -E + 3PV$$

K_t is the total molecular kinetic energy, and is the sum of the nuclear kinetic energy and of the electronic kinetic energy. Since the nuclear mass is much greater than the electronic mass, it has been supposed that the great bulk of the pressure variation in the total kinetic energy is that which is due to the variation of the electronic kinetic energy. Further, the nuclear kinetic energy is more nearly independant of temperature at high temperatures (the classical equipartition of energy is more nearly true), and it is for this reason that the highest temperatures for which results are available are chosen for the comparison. In the intercomparison of the pressure variation of the internuclear distance, direct contradiction is found. However, this may

be caused entirely by the choice of variational wave function, and not
at all by the model itself.

Certainly one of the great deficiencies of the model is the complete
neglect of temperature, and indeed it is difficult to envisage the
introduction of temperature: effects. Perhaps one could consider the gas
as a collection of rigid spheroids, the sizes of which would vary with
pressure. Kihara [26]) has considered gaseous hydrogen to consist of
rigid spheroids of fixed size, and has obtained excellent agreement
with the experimental temperature variation of the second virial
coefficient. However, a melding of the two treatments would require a
postulated pressure dependance of the size of the spheroids.

It is therefore apparent that whilst the model examined here
could yield rough qualitative agreement with experiment, a very much
more sophisticated one will be needed before quantitative agreement is
obtained.

6. APPENDIX 1 : TABLES OF RESULTS

TABLE 1

RESULTS OF A FOUR TERM NEUMANN EXPANSION

ξ_0	2α	2β	SINGLET ENERGY (au)	TRIPLET ENERGY (au)	INTERNUCLEAR DISTANCE (au)
∞	1.7235	1.3605	−1.1492453	3.4542445	1.42088
40.0	1.6715	1.3625	−1.1491880	3.4594457	1.42193
30.0	1.6525	1.3615	−1.1491632	3.4557733	1.42204
20.0	1.6125	1.3630	−1.1490314	3.4585041	1.42318
15.0	1.5690	1.3650	−1.1487877	3.4616291	1.42491
10.0	1.4745	1.3745	−1,1475591	3.4757307	1.43502
8.0	1.4070	1.3945	−1.1450026	3.5060489	1.45890
6.7	1.3585	1.4350	−1.1395302	3.5637755	1.50845
5.7	1.3400	1.5130	−1.1286463	3.6568916	1.60278
5.0	1.3545	1.6165	−1.1133526	3.7401005	1.79292
4.0	1.4650	1.9270	−1.0710889	3.8220619	2.09557

TABLE 2

RESULTS OF A FIVE TERM NEUMANN EXPANSION

ξ_0	2α	2β	SINGLET ENERGY (au)	TRIPLET ENERGY (au)	INTERNUCLEAR DISTANCE (au)
∞	1.7245	1.3615	−1.1492315	3.4567954	1.42166
40.0	1.6715	1.3625	−1.1491680	3.4594457	1.42183
30.0	1.6525	1.3615	−1.1491490	3.4556842	1.42205
20.0	1.6125	1.3640	−1.1490171	3.4616571	1.42330
10.0	1.4745	1.3745	−1.1475444	3.4756395	1.43503
8.0	1.4070	1.3945	−1.1449868	3.5059526	1.45891
6.7	1.3585	1.4350	−1.1395122	3.5636673	1.50846
5.7	1.3410	1.5130	−1.1286225	3.6564332	1.60335
5.0	1.3545	1.6165	−1.1133196	3.7399214	1.72923
4.0	1.4650	1.9260	−1.0710145	3.8210315	2.09539

TABLE 3

PRESSURE VARIATION OF THE GROUND STATE ENERGY, E,

AND OF THE INTERNAL ELECTRONIC KINETIC ENERGY, K.

ξ_0	E au	K au	PRESSURE atmos.	ΔK kcal/mole
∞	-1.1492453	1.1492453	0.	0.
40.0	-1.1491880	1.1492518	$6.54 \ 10^{-2}$	$4.07 \ 10^{-3}$
30.0	-1.1491632	1.1493122	$3.62 \ 10^{-1}$	$4.20 \ 10^{-2}$
20.0	-1.1490314	1.1494496	3.42	$1.28 \ 10^{-1}$
15.0	-1.1487877	1.1501494	$2.64 \ 10^{1}$	$5.67 \ 10^{-1}$
10.0	-1.1475591	1.153964	$4.11 \ 10^{2}$	2.96
8.0	-1.1450026	1.165124	$2.41 \ 10^{3}$	9.96
6.7	-1.1395302	1.20073	$1.13 \ 10^{4}$	$3.23 \ 10^{1}$
5.7	-1.1286463	1.29485	$4.17 \ 10^{4}$	$9.13 \ 10^{1}$
5.0	-1.1133526	1.5574	$1.32 \ 10^{5}$	$2.56 \ 10^{2}$
4.0	-1.0710889	7.719	$2.20 \ 10^{6}$	$4.12 \ 10^{3}$

TABLE 4

PRESSURE VARIATION OF THE INTERNUCLEAR
DISTANCE, R, AND OF THE BINDING ENERGY, B.E.

PRESSURE atmos.	B.E. ev	PRESSURE atmos.	R au
0.	4.061	0.	1.42088
$1.48 \ 10^2$	4.07	$6.54 \ 10^{-2}$	1.42193
$4.03 \ 10^2$	4.08	$3.62 \ 10^{-1}$	1.42204
$1.10 \ 10^3$	4.08	3.42	1.42318
$2.98 \ 10^3$	4.08	$2.64 \ 10^1$	1.42491
$8.10 \ 10^3$	4.11	$4.11 \ 10^2$	1.43502
$2.20 \ 10^4$	4.16	$2.41 \ 10^3$	1.45890
$5.98 \ 10^4$	4.73	$1.13 \ 10^4$	1.50845
$9.89 \ 10^4$	5.20	$4.17 \ 10^4$	1.60278
		$1.32 \ 10^5$	1.79292
		$2.20 \ 10^6$	2.09557

The entries in the Pressure vs B.E. table were found by graphical means.

TABLE 5

PRESSURE VARIATION OF THE MOLECULAR QUADRUPOLE MOMENT, Q,

AND OF THE LARMOR TERM IN THE MOLAR DIAMAGNETIC SUSCEPTIBILITY, $\bar{\chi}_\ell$.

PRESSURE atmos.	$Q.10^{17}$ cm^2	χ_ℓ 10^6 cgs
0.	2.6182	3.9323
$6.54\ 10^{-2}$	2.6201	3.9301
$3.62\ 10^{-1}$	2.6255	3.9261
3.42	2.6326	3.9171
$2.64\ 10^1$	2.6463	3.9036
$4.11\ 10^2$	2.7063	3.8499
$2.41\ 10^3$	2.8263	3.8003
$1.13\ 10^4$	3.0481	3.7711
$4.17\ 10^4$	3.4434	3.7991
$1.32\ 10^5$	3.9691	3.8998
$2.20\ 10^6$	5.7306	4.3833

TABLE 6

EXPECTATION OPERATORS OF THE SINGLET STATE.

PRESSURE atm.	0.	6.54×10^{-2}	3.62×10^{-1}	3.42	2.64×10^{1}	4.11×10^{2}	2.41×10^{3}	1.13×10^{4}	4.17×10^{4}	1.32×10^{5}	2.20×10^{6}
$< 1/r_{12} >$	0.6204	0.6203	0.6205	0.6205	0.6205	0.6203	0.6184	0.6128	0.5999	0.5810	0.5217
$< n^2 >$	0.3388	0.3389	0.3388	0.3389	0.3390	0.3394	0.3400	0.3414	0.3444	0.3488	0.3658
$< n^4 >$	0.2039	0.2040	0.2039	0.2040	0.2041	0.2044	0.2049	0.2060	0.2084	0.2120	0.2260
$< \xi >$	2.1725	2.1710	2.1702	2.1676	2.1634	2.1445	2.1110	2.0551	1.9701	1.8796	1.7013
$< \xi^2 >$	5.5775	5.5673	5.5618	5.5426	5.5118	5.3795	5.1669	4.8419	4.3886	3.9432	3.1537
$< \xi^3 >$	16.940	16.882	16.848	16.729	16.537	15.753	14.607	13.014	11.003	9.200	6.364
$< \xi^4 >$	60.285	59.951	59.739	59.011	57.828	53.206	47.065	39.379	30.676	23.634	13.902
$< z^2 >$	1.0078	1.0077	1.0066	1.0048	1.0022	0.9919	0.9859	0.9911	1.0223	1.0824	1.3312
$< z^4 >$	3.5332	3.5253	3.5127	3.4812	3.4310	3.2444	3.0705	2.9509	2.9663	3.1541	4.2734
$< r^2 >$	2.4814	2.4780	2.4775	2.4718	2.4633	2.4294	2.3981	2.3797	2.3974	2.4609	2.7660
$< r^4 >$	13.667	13.626	13.577	13.441	13.224	12.411	11.598	10.906	10.560	10.705	12.672
$< r_a >$	1.5434	1.5435	1.5431	1.5424	1.5417	1.5387	1.5399	1.5500	1.5788	1.6251	1.7826
$< r_a^2 >$	2.9861	2.9854	2.9831	2.9782	2.9712	2.9442	2.9302	2.9486	3.0397	3.2084	3.8639
$< r_a^3 >$	6.8909	6.8850	6.8738	6.8467	6.8056	6.6503	6.5306	6.5137	6.7410	7.2537	9.5266
$< r_a^4 >$	18.461	18.426	18.374	18.236	18.020	17.220	16.531	16.192	16.678	18.180	25.796

intensity distribution of the Q branch. An analysis of the enhancement absorption profiles given below will explain this anomalous intensity distribution of the Q branch in H_2 - Xe mixtures.

The peaks of the S(0) and S(2) lines in pH_2 - Xe (Fig. 7) and pH_2 - Kr (Fig. 8) do not exactly correspond to the corresponding Raman frequencies and it appears that there is a considerable shift of these long-range quadrupolar components toward lower frequency. Details of analysis of the enhancement absorption profiles in binary mixtures of parahydrogen with xenon, krypton and argon are described in the next two sections. This analysis enables us to determine the shifts of the quadru- polar components in binary mixtures of parahydrogen with xenon and krypton, and their characteristic half-widths in all the three mixtures. No shift of the quadrupolar line is observed for the argon case (Fig. 9) within the experimental pressures used in the present investigation.

3.2 <u>Line-shape and relative intensities of the quadrupolar components of</u> <u>the collision-induced fundamental band of H_2.</u>

It has been found by various authors (see, for example, Kiss and Welsh (1959), Watanabe and Welsh (1967), Reddy and Kuo (1971)), from the analysis of experimental absorption profiles of the induced pure rotational and vibrational-rotational spectra of the symmetric diatomic gases and their binary mixtures with foreign gases, that the quadrupolar components as well as the overlap components, except in the vicinity of the dip of the Q branch, have essentially a dispersion line-shape modified by the Boltzmann law and that the relative intensities of the quadrupolar lines are given by Van Kranendonk's theory (1958). The asymmetry of each of the components which can be expressed by the Boltzmann law is due to the participation of the relative

TABLE 8

THE TABLE ENTRIES ARE THE GROUND STATE ENERGY VALUES (in au)

OF THE HYDROGEN MOLECULAR-ION, AS CALCULATED BY COTTRELL [6]).

ξ_0 R	1.6	1.8	2.0	2.2	2.4
8	−0.5856	−0.5984	−0.6023	−0.6006	−
7	−0.5854	−0.5983	−0.6023	−0.6006	−
6	−0.5845	−0.5979	−0.6021	−0.6005	−0.5953
5	−0.5802	−0.5957	−0.6010	−0.5999	−0.5950
4	−0.5576	−0.5829	−0.5935	−0.5954	−0.5921
3	−0.4245	−0.4962	−0.5356	−0.5561	−0.5649
2	0.554	0.223	0.006	−0.140	−0.250

The underlined energy values are the minimum for the

particular ξ_0.

7.   APPENDIX 2

DERIVATION OF A RECURSION FORMULA FOR THE W_k FUNCTIONS

In the derivation which follows, the following recursion formulae for the Legendre functions will be used:

$$P_k(x) = (P'_{k+1}(x) - xP'_k(x))/(k + 1) \tag{1}$$

$$P_{k+1}(x) = (x^2 - 1)P'_k(x)/(k + 1) + xP_k(x) \tag{2}$$

and $\qquad P_k(x)Q_{k-1}(x) - P_{k-1}(x)Q_k(x) = 1/k. \tag{3}$

Let us define

$$S(k,n) = \int_1^x e^{-ay} y^n P_k(y) \, dy$$

and $\qquad T(k,m,n) = \int_1^{\xi_0} e^{-ax} x^m Q_k(x) \, S(k,n) \, dx,$

then if (1) is substituted into the expression for $S(k,n)$, and the resulting integral integrated once by parts, we have

$$(k + 1)S(k,n) = (n + 1)S(k,n) - aS(k,n + 1)$$
$$+ e^{-ax}x^n(P_{k+1}(x) - xP_k(x)) - \int_1^x e^{-ay} y^{n-1} (n - ay) P_{k+1}(y) \, dy \tag{4}$$

Substituting (2) into the integral occurring in (4), and integrating again by parts, gives

$$(k + 1)S(k,n) = S(k,n) + e^{-ax} x^n (P_{k+1}(x) - xP_k(x))$$
$$+ (a^2 S(k,n + 2) - 2a(n + 1)S(k,n + 1) - (a^2 - n(n + 1)S(k,n)$$
$$+ 2anS(k,n - 1) - n(n - 1)S(k,n - 2))/(k + 1) + e^{-ax}x^{n-1}(x^2-1)(n-ax)P_k(x)/(k+1)$$

and therefore

$$(k + 1)T(k,m,n) = \int_1^{\xi_0} e^{-ax}x^m Q_k(x) \, (e^{-ax}x^n(P_{k+1}(x) - xP_k(x))$$
$$- e^{-ax}x^{n-1}(x^2-1)(n-ax)P_k(x)/(k+1) \, dx$$
$$+ T(k,m,n) + (a^2 T(k,m,n + 2) - 2a(n + 1)T(k,m,n + 1) + 2anT(k,m,n - 1)$$
$$- n(n - 1)T(k,m,n - 2) - (a^2 - n(n + 1)T(k,m,n)))/(k + 1) \tag{5}$$

If we follow a similar procedure, but working with the $Q_k(x)$ in the integral expression for $T(k,m,n)$, we obtain firstly,

$$(k + 1)T(k,n,m) = A + (n + 1)T(k,n,m) - aT(k,n + 1,m)$$

$$- \int_1^{\xi_0} e^{-ax} x^m P_k(x)(e^{-ax} x^n (Q_{k+1}(x) - xQ_k(x))) dx - \int_1^{\xi_0} e^{-ax} x^{n-1}(n-ax)Q_{k+1}(x) S(k,n) dx$$

where $\quad A = e^{-a\xi_0} \xi_0^n (Q_{k+1}(\xi_0) - \xi_0 Q_k(\xi_0)) \int_1^{\xi_0} e^{-ax} x^m P_k(x) \, dx,$

and lastly

$$(k + 1)T(k,n,m) = B + \int_1^{\xi_0} e^{-ax} x^m P_k(x)(e^{-ax} x^n (Q_{k+1}(x) - xQ_k(x)))$$

$$- e^{-ax} x^{n-1}(x^2-1)(n-ax)Q_k(x)/(k + 1) \, dx$$

$$+ T(k,n,m) + (a^2 T(k,n + 2,m) - 2a(n + 1)T(k,n + 1,m) + 2anT(k,n - 1,m)$$

$$- n(n - 1)T(k,n - 2,m) - (a^2 - n(n + 1)T(k,n,m)))/(k + 1) \tag{6}$$

where $\quad B = e^{-a\xi_0} \xi_0^{n-1} (\xi_0 Q_{k+1}(\xi_0) - \xi_0 Q_k(\xi_0) - (\xi_0-1)(n-a\xi_0)Q_k(\xi_0)/(k+1)$

$$x \int_1^{\xi_0} e^{-ax} x^m P_k(x) \, dx.$$

Now since

$$W_k(m,n,a,\xi_0) = \int_1^{\xi_0} \int_1^{\xi_0} e^{-a(\xi_1 + \xi_2)} Q_k \begin{vmatrix} \xi_2 \\ \xi_1 \end{vmatrix} P_k \begin{vmatrix} \xi_1 \\ \xi_2 \end{vmatrix} \xi_1^m \xi_2^n \, d\xi_1 d\xi_2$$

with the upper variables being used when $\xi_2 < \xi_1$, the lower when $\xi_1 < \xi_2$, it follows that

$$W_k(m,n,a,\xi_0) = T(k,m,n) + T(k,n,m) \tag{7}$$

If equations (5) and (6) are added together and the remaining integral simplified using (3), then using (7) and rearranging terms we obtain

$$(k(k + 1) + a^2 - n(n + 1))W_k(m,n,a,\xi_0) = B + A_{m+n}(2a,\xi_0)$$

$$+ a^2W_k(m,n + 2,a,\xi_0) - 2a(n + 1)W_k(m,n + 1,a,\xi_0)$$

$$+ 2anW_k(m,n - 1,a,\xi_0) - n(n - 1)W_k(m,n - 2,a,\xi_0) \qquad (8)$$

where $\quad A_n(a,\xi_0) = \displaystyle\int_1^{\xi_0} e^{-ax} x^n \, dx.$

Equation (8) is the desired recursion formula, and is apparently new. Using this, the W_k function may be evaluated for the complete range of m,n, if it is known for m,n = 0(1)3.

Now, Miller et al [17] list, for $\xi_0 = \infty$, the W_k functions for k = 0(1)6 and m,n = 0(1)11-k, the accuracy varying from 12 figures for k = 0 to 10 figures for k = 6, and the A_n functions for n = 0(1)16 to 14 figure accuracy. The recursion formula (8) was programmed in 12 figure arithmetic and for the entire range a = 1.0(0.5)9.0, no more than two significant figures were lost for the highest m,n pair. The formula is thus numerically stable, which is in striking contrast to those given by Kotani et al [14], Rudenberg [15] and by James and Coolidge[18].

8.   APPENDIX 3

TABLES OF THE W_k FUNCTION

The following is a short tabulation of the $W_K(M,N,A.X)$ function

for:

X = 4.0, 5.0, 5.7, 6.7, 8.0, 10.0, 15.0, 20.0, 30.0, 40.0 and ∞,

K = 0 (1) 3,

M,N = 0 (1) 4 and

A = 1.0 (0.2) 2.0.

The table entries are all of 8 figures; however, only the

following accuracy is claimed:

      K = 0,   7-8 figures,

      K = 1,   6-7 figures,

      K = 2,   4-6 figures and

      K = 3,   4-6 figures.

It will be recalled that

$$W_K(M,N,A,X) = W_K(N,M,A,X).$$

X = 4.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
0	0	0	7.1248760E-02	3.7383394E-02	2.0175926E-02
0	0	1	1.1773461E-01	5.8872174E-02	3.0484388E-02
0	0	2	2.2109145E-01	1.0425450E-01	5.1218619E-02
0	0	3	4.7540949E-01	2.1048255E-01	9.7407559E-02
0	0	4	1.1590348E+00	4.8355593E-01	2.1078158E-01
0	1	1	1.9842420E-01	9.4314800E-02	4.6741584E-02
0	1	2	3.8043237E-01	1.7018422E-01	7.9847635E-02
0	1	3	8.3369184E-01	3.4986284E-01	1.5441770E-01
0	1	4	2.0633893E+00	8.1605097E-01	3.3912070E-01
0	2	2	7.4553736E-01	3.1350596E-01	1.3900532E-01
0	2	3	1.6669078E+00	6.5754925E-01	2.7403721E-01
0	2	4	4.1926631E+00	1.5599855E+00	6.1222306E-01
0	3	3	3.7964346E+00	1.4063011E+00	5.5095126E-01
0	3	4	9.6932620E+00	3.3923966E+00	1.2528015E+00
0	4	4	2.5057442E+01	8.3022000E+00	2.8948076E+00

X = 4.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
0	0	0	1.1145020E-02	6.2758822E-03	3.5910346E-03
0	0	1	1.6251953E-02	8.8772332E-03	4.9481950E-03
0	0	2	2.6067762E-02	1.3672749E-02	7.3567940E-03
0	0	3	4.6908363E-02	2.3398959E-02	1.2036599E-02
0	0	4	9.5726291E-02	4.5149947E-02	2.2040535E-02
0	1	1	2.3998296E-02	1.2692240E-02	6.8813080E-03
0	1	2	3.9053737E-02	1.9795129E-02	1.0342332E-02
0	1	3	7.1348735E-02	3.4336868E-02	1.7124273E-02
0	1	4	1.4765624E-01	6.7123107E-02	3.1732114E-02
0	2	2	6.4635400E-02	3.1334166E-02	1.5746470E-02
0	2	3	1.2020886E-01	5.5238063E-02	2.6450841E-02
0	2	4	2.5295833E-01	1.0969894E-01	4.9735159E-02
0	3	3	2.2784906E-01	9.9124244E-02	4.5160292E-02
0	3	4	4.8814072E-01	2.0033566E-01	8.6338820E-02
0	4	4	1.0638075E+00	4.1201916E-01	1.6792889E-01

X =   5.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
0	0	0	7.3151160E-02	3.7931828E-02	2.0337704E-02
0	0	1	1.2371096E-01	6.0560916E-02	3.0974022E-02
0	0	2	2.4352182E-01	1.1054570E-01	5.3031409E-02
0	0	3	5.6750550E-01	2.3625552E-01	1.0481996E-01
0	0	4	1.5536444E+00	5.9385855E-01	2.4246656E-01
0	1	1	2.1418670E-01	9.8580332E-02	4.7931692E-02
0	1	2	4.3259710E-01	1.8395211E-01	8.3604406E-02
0	1	3	1.0325456E+00	4.0180759E-01	1.6846851E-01
0	1	4	2.8806095E+00	1.0287469E+00	3.9649243E-01
0	2	2	8.9882360E-01	3.5206574E-01	1.4906454E-01
0	2	3	2.2031597E+00	7.8878297E-01	3.0740086E-01
0	2	4	6.2788296E+00	2.0639703E+00	7.3889545E-01
0	3	3	5.5378906E+00	1.8131436E+00	6.4972678E-01
0	3	4	1.6109297E+01	4.8514941E+00	1.5977580E+00
0	4	4	4.7665956E+01	1.3240611E+01	4.0142846E+00

X =   5.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
0	0	0	1.1193675E-02	6.2907576E-03	3.5956476E-03
0	0	1	1.6397045E-02	8.9210294E-03	4.9616250E-03
0	0	2	2.6602136E-02	1.3833328E-02	7.4058420E-03
0	0	3	4.9089666E-02	2.4053370E-02	1.2236158E-02
0	0	4	1.0503793E-01	4.7939319E-02	2.2889719E-02
0	1	1	2.4339228E-02	1.2792148E-02	6.9111600E-03
0	1	2	4.0109083E-02	2.0099152E-02	1.0431831E-02
0	1	3	7.5267070E-02	3.5458727E-02	1.7452805E-02
0	1	4	1.6362007E-01	7.1685311E-02	3.3065977E-02
0	2	2	6.7347166E-02	3.2086846E-02	1.5960800E-02
0	2	3	1.2899287E-01	5.7624712E-02	2.7117652E-02
0	2	4	2.8598011E-01	1.1859543E-01	5.2202966E-02
0	3	3	2.5272220E-01	1.0560378E-01	4.6901250E-02
0	3	4	5.7281035E-01	2.2186654E-01	9.1996105E-02
0	4	4	1.3270820E+00	4.7618378E-01	1.8410646E-01

X = 5.7

K	M	N	A = 1.0	A = 1.2	A = 1.4
0	0	0	7.3621020E-02	3.8043832E-02	2.0365080E-02
0	0	1	1.2541246E-01	6.0958636E-02	3.1069698E-02
0	0	2	2.5119478E-01	1.1233333E-01	5.3460523E-02
0	0	3	6.0560877E-01	2.4514753E-01	1.0695786E-01
0	0	4	1.7503487E+00	6.3984829E-01	2.5353946E-01
0	1	1	2.1902150E-01	9.9652450E-02	4.8178216E-02
0	1	2	4.51105161E-01	1.8793737E-01	8.4500506E-02
0	1	3	1.1163899E+00	4.1979822E-01	1.7249562E-01
0	1	4	3.2943063E+00	1.1175991E+00	4.1641157E-01
0	2	2	9.5849764E-01	3.6418948E-01	1.5164360E-01
0	2	3	2.4446453E+00	8.3635993E-01	3.1724492E-01
0	2	4	7.3908622E+00	2.2809000E+00	7.8343232E-01
0	3	3	6.4188638E+00	1.9766098E+00	6.8162070E-01
0	3	4	1.9876260E+01	5.5293932E+00	1.7261455E+00
0	4	4	6.2804756E+01	1.5828388E+01	4.4786120E+00

X = 5.7

K	M	N	A = 1.6	A = 1.8	A = 2.0
0	0	0	1.1200502E-02	6.2924900E-03	3.5960928E-03
0	0	1	1.6420598E-02	8.9269382E-03	4.9631305E-03
0	0	2	2.6707629E-02	1.3859764E-02	7.4125710E-03
0	0	3	4.9615968E-02	2.4185402E-02	1.2269790E-02
0	0	4	1.0776641E-01	4.8624169E-02	2.3064200E-02
0	1	1	2.4397630E-02	1.2806324E-02	6.9146720E-03
0	1	2	4.0317447E-02	2.0148951E-02	1.0444006E-02
0	1	3	7.6200608E-02	3.5681395E-02	1.7507168E-02
0	1	4	1.6824538E-01	7.2790361E-02	3.3336148E-02
0	2	2	6.7918112E-02	3.2217568E-02	1.5991589E-02
0	2	3	1.3111973E-01	5.8101607E-02	2.7227991E-02
0	2	4	2.9554684E-01	1.2073167E-01	5.2695800E-02
0	3	3	2.5924144E-01	1.0699306E-01	4.7208298E-02
0	3	4	5.9833238E-01	2.2716975E-01	9.3142220E-02
0	4	4	1.4144826E+00	4.9340310E-01	1.8764475E-01

X = 6.7

K	M	N	A = 1.0	A = 1.2	A = 1.4
0	0	0	7.3876600E-02	3.8095542E-02	2.0375850E-02
0	0	1	1.2644426E-01	6.1163209E-02	3.1111619E-02
0	0	2	2.5657088E-01	1.1339650E-01	5.3678001E-02
0	0	3	6.3663539E-01	2.5129209E-01	1.0821602E-01
0	0	4	1.9362653E+00	6.7669822E-01	2.6108607E-01
0	1	1	2.2209340E-01	1.0022618E-01	4.8290084E-02
0	1	2	4.6412871E-01	1.9031080E-01	8.4952614E-02
0	1	3	1.1847609E+00	4.3213954E-01	1.7483818E-01
0	1	4	3.6856318E+00	1.1883372E+00	4.2986017E-01
0	2	2	1.0035310E+00	3.7179170E-01	1.5300271E-01
0	2	3	2.6485361E+00	8.6959289E-01	3.2300882E-01
0	2	4	8.4677334E+00	2.4547255E+00	8.1337272E-01
0	3	3	7.2262424E+00	2.0987810E+00	7.0137204E-01
0	3	4	2.3758867E+01	6.0956961E+00	1.8146130E+00
0	4	4	8.0037056E+01	1.8181271E+01	4.8222104E+00

X = 6.7

K	M	N	A = 1.6	A = 1.8	A = 2.0
0	0	0	1.1202797E-02	6.2929866E-03	3.5962024E-03
0	0	1	1.6429413E-02	8.9288293E-03	4.9635430E-03
0	0	2	2.6753298E-02	1.3869556E-02	7.4147045E-03
0	0	3	4.9880303E-02	2.4242080E-02	1.2282144E-02
0	0	4	1.0935134E-01	4.8963748E-02	2.3138143E-02
0	1	1	2.4420202E-02	1.2811005E-02	6.9156630E-03
0	1	2	4.0406946E-02	2.0167222E-02	1.0447827E-02
0	1	3	7.6663271E-02	3.5775696E-02	1.7526874E-02
0	1	4	1.7090528E-01	7.3333051E-02	3.3449637E-02
0	2	2	6.8172874E-02	3.2267212E-02	1.6001569E-02
0	2	3	1.3217291E-01	5.8302494E-02	2.7267670E-02
0	2	4	3.0099209E-01	1.2176710E-01	5.2899911E-02
0	3	3	2.6262660E-01	1.0760301E-01	4.7322904E-02
0	3	4	6.1303605E-01	2.2974906E-01	9.3615875E-02
0	4	4	1.4679501E+00	5.0221786E-01	1.8917382E-01

X = 8.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
0	0	0	7.3968580E-02	3.8110486E-02	2.0378360E-02
0	0	1	1.2686649E-01	6.1230437E-02	3.1122722E-02
0	0	2	2.5918121E-01	1.1381148E-01	5.3746458E-02
0	0	3	6.5457407E-01	2.5414655E-01	1.0868694E-01
0	0	4	2.0638843E+00	6.9699593E-01	2.6443058E-01
0	1	1	2.2340824E-01	1.0042215E-01	4.8320770E-02
0	1	2	4.7048189E-01	1.9123028E-01	8.5093284E-02
0	1	3	1.2239663E+00	4.3779342E-01	1.7570138E-01
0	1	4	3.9524310E+00	1.2268876E+00	4.3575467E-01
0	2	2	1.0267760E+00	3.7488528E-01	1.5344372E-01
0	2	3	2.7680533E+00	8.8490414E-01	3.2512433E-01
0	2	4	9.2086024E+00	2.5488902E+00	8.2632149E-01
0	3	3	7.7393098E+00	2.1588242E+00	7.0901660E-01
0	3	4	2.6570549E+01	6.4110524E+00	1.8532881E+00
0	4	4	9.3840114E+01	1.9604476E+01	4.9829450E+00

X = 8.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
0	0	0	1.1203228E-02	6.2930622E-03	3.5962152E-03
0	0	1	1.6431299E-02	8.9291566E-03	4.9636010E-03
0	0	2	2.6764912E-02	1.3871568E-02	7.4150600E-03
0	0	3	4.9960160E-02	2.4255918E-02	1.2284586E-02
0	0	4	1.0991755E-01	4.9061678E-02	2.3155387E-02
0	1	1	2.4425192E-02	1.2811841E-02	6.9158070E-03
0	1	2	4.0429405E-02	2.0170926E-02	1.0448456E-02
0	1	3	7.6800900E-02	3.5798382E-02	1.7530719E-02
0	1	4	1.7184589E-01	7.3488160E-02	3.3475903E-02
0	2	2	6.8239250E-02	3.2277632E-02	1.6003264E-02
0	2	3	1.3248332E-01	5.8350246E-02	2.7275308E-02
0	2	4	3.0288687E-01	1.2205817E-01	5.2946407E-02
0	3	3	2.6367066E-01	1.0775400E-01	4.7345804E-02
0	3	4	6.1815258E-01	2.3046957E-01	9.3722710E-02
0	4	4	1.4876371E+00	5.0480302E-01	1.8953396E-01

X = 10.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
0	0	0	7.3993320E-02	3.8113498E-02	2.0378736E-02
0	0	1	1.2699831E-01	6.1246136E-02	3.1124669E-02
0	0	2	2.6017313E-01	1.1392930E-01	5.3761039E-02
0	0	3	6.6288022E-01	2.5513091E-01	1.0880849E-01
0	0	4	2.1356396E+00	7.0546512E-01	2.6547204E-01
0	1	1	2.2383592E-01	1.0046960E-01	4.8326332E-02
0	1	2	4.7287052E-01	1.9148738E-01	8.5122756E-02
0	1	3	1.2418302E+00	4.3970967E-01	1.7592062E-01
0	1	4	4.1006734E+00	1.2427860E+00	4.3757205E-01
0	2	2	1.0360014E+00	3.7578928E-01	1.5353975E-01
0	2	3	2.8227585E+00	8.9005320E-01	3.2565446E-01
0	2	4	9.6170752E+00	2.5870881E+00	8.3024023E-01
0	3	3	7.9919522E+00	2.1802010E+00	7.1102494E-01
0	3	4	2.8168874E+01	6.5400142E+00	1.8649386E+00
0	4	4	1.0246640E+02	2.0231110E+01	5.0343272E+00

X = 10.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
0	0	0	1.1203277E-02	6.2930688E-03	3.5962166E-03
0	0	1	1.6431548E-02	8.9291899E-03	4.9636060E-03
0	0	2	2.6766776E-02	1.3871816E-02	7.4150940E-03
0	0	3	4.9975670E-02	2.4257951E-02	1.2284859E-02
0	0	4	1.1004982E-01	4.9078930E-02	2.3157688E-02
0	1	1	2.4425872E-02	1.2811928E-02	6.9158190E-03
0	1	2	4.0432949E-02	2.0171374E-02	1.0448515E-02
0	1	3	7.6827236E-02	3.5801674E-02	1.7531144E-02
0	1	4	1.7206381E-01	7.3515301E-02	3.3479387E-02
0	2	2	6.8250112E-02	3.2278934E-02	1.6003427E-02
0	2	3	1.3254180E-01	5.8357070E-02	2.7276139E-02
0	2	4	3.0331809E-01	1.2210829E-01	5.2952484E-02
0	3	3	2.6387566E-01	1.0777636E-01	4.7348372E-02
0	3	4	6.1930421E-01	2.3059186E-01	9.3736445E-02
0	4	4	1.4922950E+00	5.0526134E-01	1.8958212E-01

X = 15.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
0	0	0	7.3996380E-02	3.8113734E-02	2.0378756E-02
0	0	1	1.2701800E-01	6.1247638E-02	3.1124792E-02
0	0	2	2.6036319E-01	1.1394370E-01	5.3762200E-02
0	0	3	6.6491866E-01	2.5528359E-01	1.0882067E-01
0	0	4	2.1581449E+00	7.0712598E-01	2.6560281E-01
0	1	1	2.2390244E-01	1.0047431E-01	4.8326700E-02
0	1	2	4.7331831E-01	1.9151809E-01	8.5125049E-02
0	1	3	1.2461219E+00	4.4000143E-01	1.7594226E-01
0	1	4	4.1465393E+00	1.2458713E+00	4.3779847E-01
0	2	2	1.0378229E+00	3.7590208E-01	1.5354751E-01
0	2	3	2.8357162E+00	8.9082162E-01	3.2570560E-01
0	2	4	9.7406117E+00	2.5943318E+00	8.3071845E-01
0	3	3	8.0560456E+00	2.1835690E+00	7.1122782E-01
0	3	4	2.8654254E+01	6.5641899E+00	1.8663352E+00
0	4	4	1.0533343E+02	2.0356916E+01	5.0408400E+00

X = 15.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
0	0	0	1.1203280E-02	6.2930688E-03	3.5962166E-03
0	0	1	1.6431559E-02	8.9291910E-03	4.9636060E-03
0	0	2	2.6766874E-02	1.3871823E-02	7.4150950E-03
0	0	3	4.9976682E-02	2.4258036E-02	1.2284866E-02
0	0	4	1.1006061E-01	4.9079849E-02	2.3157768E-02
0	1	1	2.4425900E-02	1.2811932E-02	6.9158200E-03
0	1	2	4.0433127E-02	2.0171388E-02	1.0448515E-02
0	1	3	7.6828927E-02	3.5801814E-02	1.7531154E-02
0	1	4	1.7208149E-01	7.3516753E-02	3.3479505E-02
0	2	2	6.8250674E-02	3.2278974E-02	1.6003427E-02
0	2	3	1.3254548E-01	5.8357347E-02	2.7276154E-02
0	2	4	3.0335243E-01	1.2211091E-01	5.2952679E-02
0	3	3	2.6388912E-01	1.0777732E-01	4.7348430E-02
0	3	4	6.1939407E-01	2.3059812E-01	9.3736880E-02
0	4	4	1.4926766E+00	5.0528592E-01	1.8958378E-01

X = 20.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
0	0	0	7.3996400E-02	3.8113734E-02	2.0378756E-02
0	0	1	1.2701814E-01	6.1247640E-02	3.1124792E-02
0	0	2	2.6036504E-01	1.1394374E-01	5.3762200E-02
0	0	3	6.6494754E-01	2.5528438E-01	1.0882069E-01
0	0	4	2.1586061E+00	7.0713869E-01	2.6560323E-01
0	1	1	2.2390286E-01	1.0047428E-01	4.8326684E-02
0	1	2	4.7332240E-01	1.9151811E-01	8.5125028E-02
0	1	3	1.2461809E+00	4.4000274E-01	1.7594224E-01
0	1	4	4.1474666E+00	1.2458941E+00	4.3779900E-01
0	2	2	1.0378407E+00	3.7590232E-01	1.5354750E-01
0	2	3	2.8358877E+00	8.9082507E-01	3.2570563E-01
0	2	4	9.7430275E+00	2.5943842E+00	8.3071969E-01
0	3	3	8.0569612E+00	2.1835860E+00	7.1122804E-01
0	3	4	2.8663472E+01	6.5643598E+00	1.8663387E+00
0	4	4	1.0539320E+02	2.0357880E+01	5.0408594E+00

X = 20.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
0	0	0	1.1203280E-02	6.2930688E-03	3.5962166E-03
0	0	1	1.6431559E-02	8.9291910E-03	4.9636060E-03
0	0	2	2.6766876E-02	1.3871823E-02	7.4150950E-03
0	0	3	4.9976689E-02	2.4258038E-02	1.2284867E-02
0	0	4	1.1006065E-01	4.9079853E-02	2.3157770E-02
0	1	1	2.4425896E-02	1.2811928E-02	6.9158180E-03
0	1	2	4.0433124E-02	2.0171385E-02	1.0448514E-02
0	1	3	7.6828925E-02	3.5801806E-02	1.7531150E-02
0	1	4	1.7208150E-01	7.3516736E-02	3.3479500E-02
0	2	2	6.8250674E-02	3.2278972E-02	1.6003427E-02
0	2	3	1.3254549E-01	5.8357342E-02	2.7276153E-02
0	2	4	3.0335248E-01	1.2211090E-01	5.2952672E-02
0	3	3	2.6388918E-01	1.0777730E-01	4.7348426E-02
0	3	4	6.1939425E-01	2.3059809E-01	9.3736860E-02
0	4	4	1.4926771E+00	5.0528590E-01	1.8958369E-01

X = 30.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
0	0	0	7.3996400E-02	3.8113734E-02	2.0378756E-02
0	0	1	1.2701814E-01	6.1247640E-02	3.1124792E-02
0	0	2	2.6036504E-01	1.1394374E-01	5.3762200E-02
0	0	3	6.6494779E-01	2.5528438E-01	1.0882067E-01
0	0	4	2.1586126E+00	7.0713872E-01	2.6560316E-01
0	1	1	2.2390292E-01	1.0047431E-01	4.8326700E-02
0	1	2	4.7332253E-01	1.9151818E-01	8.5125049E-02
0	1	3	1.2461818E+00	4.4000291E-01	1.7594228E-01
0	1	4	4.1474817E+00	1.2458947E+00	4.3779907E-01
0	2	2	1.0378410E+00	3.7590246E-01	1.5354751E-01
0	2	3	2.8358902E+00	8.9082542E-01	3.2570564E-01
0	2	4	9.7430655E+00	2.5943855E+00	8.3071967E-01
0	3	3	8.0569734E+00	2.1835870E+00	7.1122800E-01
0	3	4	2.8663609E+01	6.5643629E+00	1.8663385E+00
0	4	4	1.0539403E+02	2.0357890E+01	5.0408580E+00

X = 30.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
0	0	0	1.1203280E-02	6.2930688E-03	3.5962166E-03
0	0	1	1.6431559E-02	8.9291910E-03	4.9636060E-03
0	0	2	2.6766875E-02	1.3871823E-02	7.4150950E-03
0	0	3	4.9976689E-02	2.4258036E-02	1.2284866E-02
0	0	4	1.1006065E-01	4.9079849E-02	2.3157766E-02
0	1	1	2.4425902E-02	1.2811932E-02	6.9158200E-03
0	1	2	4.0433133E-02	2.0171388E-02	1.0448515E-02
0	1	3	7.6828950E-02	3.5801814E-02	1.7531153E-02
0	1	4	1.7208156E-01	7.3516753E-02	3.3479502E-02
0	2	2	6.8250686E-02	3.2278974E-02	1.6003427E-02
0	2	3	1.3254551E-01	5.8357347E-02	2.7276153E-02
0	2	4	3.0335255E-01	1.2211091E-01	5.2952674E-02
0	3	3	2.6388922E-01	1.0777732E-01	4.7348426E-02
0	3	4	6.1939441E-01	2.3059812E-01	9.3736865E-02
0	4	4	1.4926778E+00	5.0528592E-01	1.8958371E-01

X = 40.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
0	0	0	7.3996400E-02	3.8113734E-02	2.0378756E-02
0	0	1	1.2701814E-01	6.1247640E-02	3.1124792E-02
0	0	2	2.6036504E-01	1.1394374E-01	5.3762200E-02
0	0	3	6.6494779E-01	2.5528438E-01	1.0882067E-01
0	0	4	2.1586126E+00	7.0713872E-01	2.6560316E-01
0	1	1	2.2390292E-01	1.0047431E-01	4.8326700E-02
0	1	2	4.7332253E-01	1.9151818E-01	8.5125049E-02
0	1	3	1.2461818E+00	4.4000291E-01	1.7594228E-01
0	1	4	4.1474817E+00	1.2458947E+00	4.3779907E-01
0	2	2	1.0378410E+00	3.7590246E-01	1.5354751E-01
0	2	3	2.8358902E+00	8.9082542E-01	3.2570564E-01
0	2	4	9.7430655E+00	2.5943855E+00	8.3071967E-01
0	3	3	8.0569734E+00	2.1835870E+00	7.1122800E-01
0	3	4	2.8663611E+01	6.5643629E+00	1.8663385E+00
0	4	4	1.0539413E+02	2.0357890E+01	5.0408580E+00

X = 40.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
0	0	0	1.1203280E-02	6.2930688E-03	3.5962166E-03
0	0	1	1.6431559E-02	8.9291910E-03	4.9636060E-03
0	0	2	2.6766875E-02	1.3871823E-02	7.4150950E-03
0	0	3	4.9976689E-02	2.4258036E-02	1.2284866E-02
0	0	4	1.1006065E-01	4.9079849E-02	2.3157766E-02
0	1	1	2.4425902E-02	1.2811932E-02	6.9158200E-03
0	1	2	4.0433133E-02	2.0171388E-02	1.0448515E-02
0	1	3	7.6828950E-02	3.5801814E-02	1.7531153E-02
0	1	4	1.7208156E-01	7.3516753E-02	3.3479502E-02
0	2	2	6.8250686E-02	3.2278974E-02	1.6003427E-02
0	2	3	1.3254551E-01	5.8357347E-02	2.7276153E-02
0	2	4	3.0335255E-01	1.2211091E-01	5.2952674E-02
0	3	3	2.6388922E-01	1.0777732E-01	4.7348426E-02
0	3	4	6.1939441E-01	2.3059812E-01	9.3736865E-02
0	4	4	1.4926778E+00	5.0528592E-01	1.8958371E-01

X = ∞

K	M	N	A = 1.0	A = 1.2	A = 1.4
0	0	0	7.3996400E-02	3.8113734E-02	2.0378756E-02
0	0	1	1.2701814E-01	6.1247640E-02	3.1124792E-02
0	0	2	2.6036504E-01	1.1394374E-01	5.3762200E-02
0	0	3	6.6494779E-01	2.5528438E-01	1.0882067E-01
0	0	4	2.1586126E+00	7.0713872E-01	2.6560316E-01
0	1	1	2.2390292E-01	1.0047431E-01	4.8326700E-02
0	1	2	4.7332253E-01	1.9151818E-01	8.5125049E-02
0	1	3	1.2461818E+00	4.4000291E-01	1.7594228E-01
0	1	4	4.1474817E+00	1.2458947E+00	4.3779907E-01
0	2	2	1.0378410E+00	3.7590246E-01	1.5354751E-01
0	2	3	2.8358902E+00	8.9082542E-01	3.2570564E-01
0	2	4	9.7430655E+00	2.5943855E+00	8.3071967E-01
0	3	3	8.0569734E+00	2.1835870E+00	7.1122800E-01
0	3	4	2.8663611E+01	6.5643629E+00	1.8663385E+00
0	4	4	1.0539413E+02	2.0357890E+01	5.0408580E+00

X = ∞

K	M	N	A = 1.6	A = 1.8	A = 2.0
0	0	0	1.1203280E-02	6.2930688E-03	3.5962166E-03
0	0	1	1.6431559E-02	8.9291910E-03	4.9636060E-03
0	0	2	2.6766875E-02	1.3871823E-02	7.4150950E-03
0	0	3	4.9976689E-02	2.4258036E-02	1.2284866E-02
0	0	4	1.1006065E-01	4.9079849E-02	2.3157766E-02
0	1	1	2.4425902E-02	1.2811932E-02	6.9158200E-03
0	1	2	4.0433133E-02	2.0171388E-02	1.0448515E-02
0	1	3	7.6828950E-02	3.5801814E-02	1.7531153E-02
0	1	4	1.7208156E-01	7.3516753E-02	3.3479502E-02
0	2	2	6.8250686E-02	3.2278974E-02	1.6003427E-02
0	2	3	1.3254551E-01	5.8357347E-02	2.7276153E-02
0	2	4	3.0335255E-01	1.2211091E-01	5.2952674E-02
0	3	3	2.6388922E-01	1.0777732E-01	4.7348426E-02
0	3	4	6.1939441E-01	2.3059812E-01	9.3736865E-02
0	4	4	1.4926778E+00	5.0528592E-01	1.8958371E-01

X = 4.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
1	0	0	2.0528108E-02	1.1131556E-02	6.1952556E-03
1	0	1	3.2185176E-02	1.6641916E-02	8.9035642E-03
1	0	2	5.6615292E-02	2.7559890E-02	1.4002230E-02
1	0	3	1.1331262E-01	5.1491121E-02	2.4585204E-02
1	0	4	2.5782911E-01	1.0930997E-01	4.8821008E-02
1	1	1	5.2696206E-02	2.5801236E-02	1.3188904E-02
1	1	2	9.7308690E-02	4.4581132E-02	2.1507963E-02
1	1	3	2.0435603E-01	8.7089899E-02	3.9300397E-02
1	1	4	4.8483913E-01	1.9267908E-01	8.1156197E-02
1	2	2	1.8935074E-01	8.0832082E-02	3.6605042E-02
1	2	3	4.1793470E-01	1.6581219E-01	7.0015576E-02
1	2	4	1.0339701E+00	3.8329614E-01	1.5103382E-01
1	3	3	9.6528040E-01	3.5673324E-01	1.4041067E-01
1	3	4	2.4783886E+00	8.5952011E-01	3.1643352E-01
1	4	4	6.5567676E+00	2.1451714E+00	7.4174980E-01

X = 4.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
1	0	0	3.5202662E-03	2.0340954E-03	1.1915888E-03
1	0	1	4.8957062E-03	2.7520541E-03	1.5750774E-03
1	0	2	7.3690712E-03	3.9915712E-03	2.2137081E-03
1	0	3	1.2248454E-02	6.3255255E-03	3.3665041E-03
1	0	4	2.2854387E-02	1.1152410E-02	5.6420538E-03
1	1	1	6.9821886E-03	3.8027088E-03	2.1193034E-03
1	1	2	1.0837012E-02	5.6599088E-03	3.0443983E-03
1	1	3	1.8651606E-02	9.2431088E-03	4.7506795E-03
1	1	4	3.6073030E-02	1.6828520E-02	8.1908840E-03
1	2	2	1.7453905E-02	8.6948366E-03	4.4926070E-03
1	2	3	3.1305834E-02	1.4725286E-02	7.2354930E-03
1	2	4	6.3117217E-02	2.7855974E-02	1.2911837E-02
1	3	3	5.8727076E-02	2.5982634E-02	1.2087385E-02
1	3	4	1.2371758E-01	5.1270079E-02	2.2432262E-02
1	4	4	2.7175072E-01	1.0553782E-01	4.3375478E-02

X =   5.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
1	0	0	2.0803742E-02	1.1206745E-02	6.2163942E-03
1	0	1	3.3091649E-02	1.6883159E-02	8.9699063E-03
1	0	2	6.0043864E-02	2.8463005E-02	1.4248482E-02
1	0	3	1.2728425E-01	5.5158465E-02	2.5582299E-02
1	0	4	3.1703989E-01	1.2482690E-01	5.3034709E-02
1	1	1	5.5347712E-02	2.6474254E-02	1.3365951E-02
1	1	2	1.0652253E-01	4.6857020E-02	2.2091673E-02
1	1	3	2.3991830E-01	9.5763249E-02	4.1499624E-02
1	1	4	6.3050207E-01	2.2799936E-01	9.0071017E-02
1	2	2	2.1910298E-01	8.7852400E-02	3.8325830E-02
1	2	3	5.2676538E-01	1.9082064E-01	7.5986307E-02
1	2	4	1.4636301E+00	4.8063073E-01	1.7396575E-01
1	3	3	1.3462558E+00	4.4087922E-01	1.5968464E-01
1	3	4	3.9340080E+00	1.1733819E+00	3.8657471E-01
1	4	4	1.1975132E+01	3.2760076E+00	9.8576770E-01

X =   5.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
1	0	0	3.5263650E-03	2.0358952E-03	1.1921293E-03
1	0	1	4.9144749E-03	2.7574992E-03	1.5766913E-03
1	0	2	7.4382387E-03	4.0115161E-03	2.2195867E-03
1	0	3	1.2527961E-02	6.4059844E-03	3.3901852E-03
1	0	4	2.4034385E-02	1.1491737E-02	5.7418290E-03
1	1	1	7.0302836E-03	3.8161488E-03	2.1231608E-03
1	1	2	1.0991913E-02	5.7023027E-03	3.0563309E-03
1	1	3	1.9229583E-02	9.3999938E-03	4.7945180E-03
1	1	4	3.8407644E-02	1.7460525E-02	8.3671070E-03
1	2	2	1.7890930E-02	8.8095866E-03	4.5236720E-03
1	2	3	3.2784494E-02	1.5104418E-02	7.3358830E-03
1	2	4	6.8728181E-02	2.9279273E-02	1.3285190E-02
1	3	3	6.3303784E-02	2.7108044E-02	1.2373473E-02
1	3	4	1.3996573E-01	5.5169294E-02	2.3400438E-02
1	4	4	3.2622550E-01	1.1811967E-01	4.6380530E-02

X = 5.7

K	M	N	A = 1.0	A = 1.2	A = 1.4
1	0	0	2.0861692E-02	1.1219650E-02	6.2193656E-03
1	0	1	3.3312357E-02	1.6930999E-02	8.9806807E-03
1	0	2	6.1043716E-02	2.8678349E-02	1.4296789E-02
1	0	3	1.3220298E-01	5.6218404E-02	2.5820609E-02
1	0	4	3.4216665E-01	1.3025384E-01	5.4257620E-02
1	1	1	5.6060450E-02	2.6619628E-02	1.3396940E-02
1	1	2	1.0939993E-01	4.7426236E-02	2.2209732E-02
1	1	3	2.5313220E-01	9.8350550E-02	4.2032445E-02
1	1	4	6.9533201E-01	2.4067767E-01	9.2682366E-02
1	2	2	2.2958100E-01	8.9805232E-02	3.8707908E-02
1	2	3	5.7146099E-01	1.9889824E-01	7.7521306E-02
1	2	4	1.6725075E+00	5.1791776E-01	1.8097605E-01
1	3	3	1.5255042E+00	4.7165150E-01	1.6522818E-01
1	3	4	4.7343573E+00	1.3070959E+00	4.0999555E-01
1	4	4	1.5418730E+01	3.8284738E+00	1.0783011E+00

X = 5.7

K	M	N	A = 1.6	A = 1.8	A = 2.0
1	0	0	3.5270724E-03	2.0360646E-03	1.1921723E-03
1	0	1	4.9169862E-03	2.7580990E-03	1.5768400E-03
1	0	2	7.4494818E-03	4.0141997E-03	2.2202468E-03
1	0	3	1.2583480E-02	6.4192750E-03	3.3934484E-03
1	0	4	2.4319792E-02	1.1560190E-02	5.7586432E-03
1	1	1	7.0371574E-03	3.8177300E-03	2.1235376E-03
1	1	2	1.1017506E-02	5.7080610E-03	3.0576721E-03
1	1	3	1.9344383E-02	9.4257143E-03	4.8004765E-03
1	1	4	3.8970870E-02	1.7586887E-02	8.3964120E-03
1	2	2	1.7969342E-02	8.8263476E-03	4.5273950E-03
1	2	3	3.3090758E-02	1.5168261E-02	7.3497310E-03
1	2	4	7.0114393E-02	2.9566216E-02	1.3347085E-02
1	3	3	6.4351086E-02	2.7315092E-02	1.2416155E-02
1	3	4	1.4426819E-01	5.5997213E-02	2.3566852E-02
1	4	4	3.4243040E-01	1.2108753E-01	4.6948250E-02

X =   6.7

K	M	N	A = 1.0	A = 1.2	A = 1.4
1	0	0	2.0889408E-02	1.1224825E-02	6.2203784E-03
1	0	1	3.3429970E-02	1.6952414E-02	8.9847870E-03
1	0	2	6.1655504E-02	2.8789099E-02	1.4317883E-02
1	0	3	1.3569101E-01	5.6851833E-02	2.5941578E-02
1	0	4	3.6282338E-01	1.3401364E-01	5.4977014E-02
1	1	1	5.6464180E-02	2.6687926E-02	1.3409181E-02
1	1	2	1.1122298E-01	4.7724593E-02	2.2261744E-02
1	1	3	2.6272540E-01	9.9907232E-02	4.2301989E-02
1	1	4	7.4970603E-01	2.4949955E-01	9.4211558E-02
1	2	2	2.3678582E-01	9.0901166E-02	3.8886192E-02
1	2	3	6.0599824E-01	2.0396671E-01	7.8317963E-02
1	2	4	1.8571222E+00	5.4465124E-01	1.8513277E-01
1	3	3	1.6783890E+00	4.9267238E-01	1.6831735E-01
1	3	4	5.5056627E+00	1.4096052E+00	4.2455711E-01
1	4	4	1.9129764E+01	4.2961096E+00	1.1410034E+00

X =   6.7

K	M	N	A = 1.6	A = 1.8	A = 2.0
1	0	0	3.5272774E-03	2.0361116E-03	1.1921810E-03
1	0	1	4.9178068E-03	2.7582726E-03	1.5768736E-03
1	0	2	7.4536150E-03	4.0150232E-03	2.2203995E-03
1	0	3	1.2607452E-02	6.4241666E-03	3.3944531E-03
1	0	4	2.4462753E-02	1.1589472E-02	5.7647493E-03
1	1	1	7.0394174E-03	3.8181466E-03	2.1235968E-03
1	1	2	1.1026982E-02	5.7098399E-03	3.0579943E-03
1	1	3	1.9393542E-02	9.4350571E-03	4.8022845E-03
1	1	4	3.9250565E-02	1.7640313E-02	8.4069155E-03
1	2	2	1.7999927E-02	8.8318300E-03	4.5283950E-03
1	2	3	3.3223686E-02	1.5191625E-02	7.3540025E-03
1	2	4	7.0802897E-02	2.9686748E-02	1.3369158E-02
1	3	3	6.4834406E-02	2.7395144E-02	1.2430094E-02
1	3	4	1.4647404E-01	5.6351918E-02	2.3627033E-02
1	4	4	3.5137612E-01	1.2244233E-01	4.7165196E-02

X = 8.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
1	0	0	2.0897900E-02	1.1226116E-02	6.2205884E-03
1	0	1	3.3470936E-02	1.6958396E-02	8.9857177E-03
1	0	2	6.1907268E-02	2.8825792E-02	1.4323539E-02
1	0	3	1.3739679E-01	5.7100258E-02	2.5979885E-02
1	0	4	3.7481521E-01	1.3576201E-01	5.5246518E-02
1	1	1	5.6613930E-02	2.6708002E-02	1.3412065E-02
1	1	2	1.1199042E-01	4.7823853E-02	2.2275548E-02
1	1	3	2.6746252E-01	1.0051398E-01	4.2386027E-02
1	1	4	7.8149666E-01	2.5357608E-01	9.4777247E-02
1	2	2	2.4007376E-01	9.1290166E-02	3.8936034E-02
1	2	3	6.2395478E-01	2.0599953E-01	7.8569064E-02
1	2	4	1.9692380E+00	5.5717581E-01	1.8666594E-01
1	3	3	1.7663146E+00	5.0182008E-01	1.6935884E-01
1	3	4	6.0135305E+00	1.4602959E+00	4.3010518E-01
1	4	4	2.1877308E+01	4.5517036E+00	1.1669850E+00

X = 8.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
1	0	0	3.5273200E-03	2.0361162E-03	1.1921819E-03
1	0	1	4.9179649E-03	2.7582932E-03	1.5768783E-03
1	0	2	7.4545424E-03	4.0151653E-03	2.2204247E-03
1	0	3	1.2613646E-02	6.4251805E-03	3.3946256E-03
1	0	4	2.4506155E-02	1.1596628E-02	5.7659658E-03
1	1	1	7.0398612E-03	3.8182032E-03	2.1236106E-03
1	1	2	1.1029036E-02	5.7101326E-03	3.0580478E-03
1	1	3	1.9405946E-02	9.4369405E-03	4.8025970E-03
1	1	4	3.9334129E-02	1.7653160E-02	8.4090085E-03
1	2	2	1.8006817E-02	8.8327866E-03	4.5285490E-03
1	2	3	3.3257193E-02	1.5196317E-02	7.3547125E-03
1	2	4	7.1006099E-02	2.9715296E-02	1.3373433E-02
1	3	3	6.4962950E-02	2.7412134E-02	1.2432476E-02
1	3	4	1.4713460E-01	5.6436564E-02	2.3638580E-02
1	4	4	3.5424912E-01	1.2278536E-01	4.7208986E-02

X = 10.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
1	0	0	2.0899828E-02	1.1226345E-02	6.2206100E-03
1	0	1	3.3481620E-02	1.6959582E-02	8.9858464E-03
1	0	2	6.1986268E-02	2.8834376E-02	1.4324489E-02
1	0	3	1.3804630E-01	5.7170730E-02	2.5987898E-02
1	0	4	3.8036509E-01	1.3636375E-01	5.5315590E-02
1	1	1	5.6655090E-02	2.6712118E-02	1.3412495E-02
1	1	2	1.1223159E-01	4.7846641E-02	2.2277770E-02
1	1	3	2.6925371E-01	1.0068336E-01	4.2403387E-02
1	1	4	7.9510463E-01	2.5496032E-01	9.4920497E-02
1	2	2	2.4118536E-01	9.1384732E-02	3.8944600E-02
1	2	3	6.3095809E-01	2.0657082E-01	7.8620578E-02
1	2	4	2.0215120E+00	5.6139599E-01	1.8704702E-01
1	3	3	1.8040114E+00	5.0459638E-01	1.6958868E-01
1	3	4	6.2656290E+00	1.4779723E+00	4.3150897E-01
1	4	4	2.3407082E+01	4.6494680E+00	1.1740732E+00

X = 10.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
1	0	0	3.5273162E-03	2.0361180E-03	1.1921831E-03
1	0	1	4.9179749E-03	2.7582995E-03	1.5768804E-03
1	0	2	7.4546461E-03	4.0151908E-03	2.2204298E-03
1	0	3	1.2614528E-02	6.4252688E-03	3.3946192E-03
1	0	4	2.4514300E-02	1.1597628E-02	5.7660727E-03
1	1	1	7.0399086E-03	3.8182232E-03	2.1236140E-03
1	1	2	1.1029219E-02	5.7101472E-03	3.0580293E-03
1	1	3	1.9407759E-02	9.4371316E-03	4.8025910E-03
1	1	4	3.9349804E-02	1.7654987E-02	8.4091800E-03
1	2	2	1.8007586E-02	8.8328688E-03	4.5285280E-03
1	2	3	3.3262139E-02	1.5196821E-02	7.3547245E-03
1	2	4	7.1043608E-02	2.9719312E-02	1.3373808E-02
1	3	3	6.4983696E-02	2.7414056E-02	1.2432622E-02
1	3	4	1.4725802E-01	5.6448221E-02	2.3639703E-02
1	4	4	3.5482262E-01	1.2283615E-01	4.7213814E-02

X = 15.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
1	0	0	2.0900010E-02	1.1226351E-02	6.2206156E-03
1	0	1	3.3482865E-02	1.6959674E-02	8.9858542E-03
1	0	2	6.1998170E-02	2.8835186E-02	1.4324581E-02
1	0	3	1.3817203E-01	5.7179466E-02	2.5988652E-02
1	0	4	3.8172667E-01	1.3645696E-01	5.5322758E-02
1	1	1	5.6660180E-02	2.6712488E-02	1.3412510E-02
1	1	2	1.1226771E-01	4.7848842E-02	2.2277962E-02
1	1	3	2.6959031E-01	1.0070374E-01	4.2404776E-02
1	1	4	7.9962181E-01	2.5517185E-01	9.4934651E-02
1	2	2	2.4136082E-01	9.1393682E-02	3.8945304E-02
1	2	3	6.3227907E-01	2.0663761E-01	7.8624828E-02
1	2	4	2.0339356E+00	5.6202150E-01	1.8708460E-01
1	3	3	1.8117938E+00	5.0494806E-01	1.6960774E-01
1	3	4	6.3276682E+00	1.4806221E+00	4.3164388E-01
1	4	4	2.3828190E+01	4.6654338E+00	1.1747984E+00

X = 15.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
1	0	0	3.5273150E-03	2.0361166E-03	1.1921833E-03
1	0	1	4.9179724E-03	2.7582974E-03	1.5768793E-03
1	0	2	7.4546462E-03	4.0151844E-03	2.2204281E-03
1	0	3	1.2614594E-02	6.4252783E-03	3.3946213E-03
1	0	4	2.4514813E-02	1.1597638E-02	5.7660518E-03
1	1	1	7.0399062E-03	3.8182176E-03	2.1236096E-03
1	1	2	1.1029221E-02	5.7101360E-03	3.0580214E-03
1	1	3	1.9407803E-02	9.4370966E-03	4.8025545E-03
1	1	4	3.9350695E-02	1.7654964E-02	8.4091125E-03
1	2	2	1.8007520E-02	8.8327944E-03	4.5284850E-03
1	2	3	3.3262221E-02	1.5196725E-02	7.3546600E-03
1	2	4	7.1045512E-02	2.9719190E-02	1.3373683E-02
1	3	3	6.4984600E-02	2.7414030E-02	1.2432543E-02
1	3	4	1.4726526E-01	5.6448502E-02	2.3639587E-02
1	4	4	3.5485948E-01	1.2283794E-01	4.7213734E-02

X = 20.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
1	0	0	2.0899980E-02	1.1226328E-02	6.2206084E-03
1	0	1	3.3482829E-02	1.6959622E-02	8.9858577E-03
1	0	2	6.1998164E-02	2.8835075E-02	1.4324582E-02
1	0	3	1.3816933E-01	5.7178051E-02	2.5988190E-02
1	0	4	3.8172637E-01	1.3645145E-01	5.5321137E-02
1	1	1	5.6660210E-02	2.6712406E-02	1.3412538E-02
1	1	2	1.1226793E-01	4.7848658E-02	2.2278002E-02
1	1	3	2.6958470E-01	1.0070085E-01	4.2403999E-02
1	1	4	7.9964220E-01	2.5516461E-01	9.4933113E-02
1	2	2	2.4136212E-01	9.1393316E-02	3.8945370E-02
1	2	3	6.3227897E-01	2.0663407E-01	7.8624035E-02
1	2	4	2.0340868E+00	5.6201898E-01	1.8708443E-01
1	3	3	1.8117692E+00	5.0492736E-01	1.6960215E-01
1	3	4	6.3281568E+00	1.4805764E+00	4.3163129E-01
1	4	4	2.3833698E+01	4.6654112E+00	1.1747797E+00

X = 20.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
1	0	0	3.5273174E-03	2.0361156E-03	1.1921814E-03
1	0	1	4.9179787E-03	2.7582983E-03	1.5768788E-03
1	0	2	7.4546593E-03	4.0151878E-03	2.2204261E-03
1	0	3	1.2614464E-02	6.4252127E-03	3.3945880E-03
1	0	4	2.4514389E-02	1.1597457E-02	5.7659666E-03
1	1	1	7.0399224E-03	3.8182200E-03	2.1236130E-03
1	1	2	1.1029252E-02	5.7101427E-03	3.0580257E-03
1	1	3	1.9407566E-02	9.4369849E-03	4.8025140E-03
1	1	4	3.9350315E-02	1.7654799E-02	8.4090675E-03
1	2	2	1.8007565E-02	8.8328132E-03	4.5284870E-03
1	2	3	3.3262031E-02	1.5196654E-02	7.3546290E-03
1	2	4	7.1045592E-02	2.9719238E-02	1.3373691E-02
1	3	3	6.4983166E-02	2.7413526E-02	1.2432374E-02
1	3	4	1.4726236E-01	5.6447602E-02	2.3639315E-02
1	4	4	3.5485538E-01	1.2283684E-01	4.7213430E-02

X = 30.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
1	0	0	2.0900000E-02	1.1226335E-02	6.2206114E-03
1	0	1	3.3482868E-02	1.6959635E-02	8.9858463E-03
1	0	2	6.1998214E-02	2.8835175E-02	1.4324547E-02
1	0	3	1.3817394E-01	5.7179635E-02	2.5988684E-02
1	0	4	3.8174474E-01	1.3645790E-01	5.5322697E-02
1	1	1	5.6660230E-02	2.6712428E-02	1.3412492E-02
1	1	2	1.1226753E-01	4.7848846E-02	2.2277888E-02
1	1	3	2.6958965E-01	1.0070409E-01	4.2404858E-02
1	1	4	7.9948454E-01	2.5517334E-01	9.4934614E-02
1	2	2	2.4135484E-01	9.1394032E-02	3.8945080E-02
1	2	3	6.3209872E-01	2.0663917E-01	7.8624914E-02
1	2	4	2.0279558E+00	5.6201957E-01	1.8708428E-01
1	3	3	1.8057658E+00	5.0494598E-01	1.6961042E-01
1	3	4	6.3013987E+00	1.4806169E+00	4.3165008E-01
1	4	4	2.3716202E+01	4.6654264E+00	1.1748081E+00

X = 30.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
1	0	0	3.5273200E-03	2.0361178E-03	1.1921825E-03
1	0	1	4.9179818E-03	2.7582980E-03	1.5768775E-03
1	0	2	7.4546687E-03	4.0151875E-03	2.2204231E-03
1	0	3	1.2614714E-02	6.4253049E-03	3.3946325E-03
1	0	4	2.4515001E-02	1.1597651E-02	5.7660465E-03
1	1	1	7.0399200E-03	3.8182166E-03	2.1236074E-03
1	1	2	1.1029249E-02	5.7101321E-03	3.0580137E-03
1	1	3	1.9407995E-02	9.4371215E-03	4.8025745E-03
1	1	4	3.9350905E-02	1.7654886E-02	8.4090750E-03
1	2	2	1.8007578E-02	8.8327822E-03	4.5284640E-03
1	2	3	3.3262599E-02	1.5196727E-02	7.3546510E-03
1	2	4	7.1045930E-02	2.9718980E-02	1.3373531E-02
1	3	3	6.4986300E-02	2.7414190E-02	1.2432645E-02
1	3	4	1.4726823E-01	5.6448572E-02	2.3639651E-02
1	4	4	3.5486122E-01	1.2283703E-01	4.7213376E-02

X = 40.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
1	0	0	2.0900000E-02	1.1226335E-02	6.2206114E-03
1	0	1	3.3482868E-02	1.6959635E-02	8.9858463E-03
1	0	2	6.1998214E-02	2.8835175E-02	1.4324547E-02
1	0	3	1.3817410E-01	5.7179635E-02	2.5988684E-02
1	0	4	3.8175062E-01	1.3645790E-01	5.5322697E-02
1	1	1	5.6660230E-02	2.6712428E-02	1.3412492E-02
1	1	2	1.1226769E-01	4.7848846E-02	2.2277888E-02
1	1	3	2.6959553E-01	1.0070409E-01	4.2404858E-02
1	1	4	7.9967700E-01	2.5517350E-01	9.4934614E-02
1	2	2	2.4136072E-01	9.1394032E-02	3.8945080E-02
1	2	3	6.3229086E-01	2.0663934E-01	7.8624914E-02
1	2	4	2.0340885E+00	5.6202877E-01	1.8708428E-01
1	3	3	1.8118916E+00	5.0495518E-01	1.6961042E-01
1	3	4	6.3285508E+00	1.4806513E+00	4.3165006E-01
1	4	4	2.3834578E+01	4.6655530E+00	1.1748080E+00

X = 40.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
1	0	0	3.5273200E-03	2.0361178E-03	1.1921825E-03
1	0	1	4.9179818E-03	2.7582980E-03	1.5768775E-03
1	0	2	7.4546687E-03	4.0151875E-03	2.2204231E-03
1	0	3	1.2614714E-02	6.4253049E-03	3.3946325E-03
1	0	4	2.4515001E-02	1.1597650E-02	5.7660465E-03
1	1	1	7.0399200E-03	3.8182166E-03	2.1236074E-03
1	1	2	1.1029249E-02	5.7101321E-03	3.0580137E-03
1	1	3	1.9407995E-02	9.4371215E-03	4.8025745E-03
1	1	4	3.9350905E-02	1.7654885E-02	8.4090750E-03
1	2	2	1.8007578E-02	8.8327822E-03	4.5284640E-03
1	2	3	3.3262599E-02	1.5196727E-02	7.3546510E-03
1	2	4	7.1045930E-02	2.9718978E-02	1.3373531E-02
1	3	3	6.4986300E-02	2.7414190E-02	1.2432645E-02
1	3	4	1.4726823E-01	5.6448567E-02	2.3639651E-02
1	4	4	3.5486122E-01	1.2283700E-01	4.7213374E-02

X = ∞

K	M	N	A = 1.0	A = 1.2	A = 1.4
1	0	0	2.0900000E-02	1.1226335E-02	6.2206114E-03
1	0	1	3.3482868E-02	1.6959635E-02	8.9858463E-03
1	0	2	6.1998214E-02	2.8835175E-02	1.4324547E-02
1	0	3	1.3817410E-01	5.7179635E-02	2.5988684E-02
1	0	4	3.8175062E-01	1.3645790E-01	5.5322697E-02
1	1	1	5.6660230E-02	2.6712428E-02	1.3412492E-02
1	1	2	1.1226769E-01	4.7848846E-02	2.2277888E-02
1	1	3	2.6959553E-01	1.0070409E-01	4.2404858E-02
1	1	4	7.9967700E-01	2.5517350E-01	9.4934614E-02
1	2	2	2.4136072E-01	9.1394032E-02	3.8945080E-02
1	2	3	6.3229086E-01	2.0663934E-01	7.8624914E-02
1	2	4	2.0340885E+00	5.6202877E-01	1.8708428E-01
1	3	3	1.8118916E+00	5.0495518E-01	1.6961042E-01
1	3	4	6.3285508E+00	1.4806513E+00	4.3165006E-01
1	4	4	2.3834578E+01	4.6655530E+00	1.1748080E+00

X = ∞

K	M	N	A = 1.6	A = 1.8	A = 2.0
1	0	0	3.5273200E-03	2.0361178E-03	1.1921825E-03
1	0	1	4.9179818E-03	2.7582980E-03	1.5768775E-03
1	0	2	7.4546687E-03	4.0151875E-03	2.2204231E-03
1	0	3	1.2614714E-02	6.4253049E-03	3.3946325E-03
1	0	4	2.4515001E-02	1.1597650E-02	5.7660465E-03
1	1	1	7.0399200E-03	3.8182166E-03	2.1236074E-03
1	1	2	1.1029249E-02	5.7101321E-03	3.0580137E-03
1	1	3	1.9407995E-02	9.4371215E-03	4.8025745E-03
1	1	4	3.9350905E-02	1.7654885E-02	8.4090750E-03
1	2	2	1.8007578E-02	8.8327822E-03	4.5284640E-03
1	2	3	3.3262599E-02	1.5196727E-02	7.3546510E-03
1	2	4	7.1045930E-02	2.9718978E-02	1.3373531E-02
1	3	3	6.4986300E-02	2.7414190E-02	1.2432645E-02
1	3	4	1.4726823E-01	5.6448567E-02	2.3639651E-02
1	4	4	3.5486122E-01	1.2283700E-01	4.7213374E-02

X = 4.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
2	0	0	9.0931070E-03	5.0029670E-03	2.8243009E-03
2	0	1	1.3926062E-02	7.2982455E-03	3.9606462E-03
2	0	2	2.3747286E-02	1.1688880E-02	6.0209980E-03
2	0	3	4.5816440E-02	2.0946298E-02	1.0116939E-02
2	0	4	1.0042351E-01	4.2460353E-02	1.9081045E-02
2	1	1	2.2664037E-02	1.1199372E-02	5.7913620E-03
2	1	2	4.1427304E-02	1.9053559E-02	9.2667770E-03
2	1	3	8.5766145E-02	3.6454818E-02	1.6504384E-02
2	1	4	2.0006553E-01	7.8705505E-02	3.3045106E-02
2	2	2	8.1591665E-02	3.4719276E-02	1.5754838E-02
2	2	3	1.8135655E-01	7.1259415E-02	2.9967514E-02
2	2	4	4.4940969E-01	1.6405044E-01	6.3987985E-02
2	3	3	4.2946038E-01	1.5642944E-01	6.0967455E-02
2	3	4	1.1202073E+00	3.8166737E-01	1.3852140E-01
2	4	4	3.0410486E+00	9.7705140E-01	3.3237444E-01

X = 4.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
2	0	0	1.6266395E-03	9.5191580E-04	5.6428625E-04
2	0	1	2.2087888E-03	1.2586658E-03	7.2972170E-04
2	0	2	3.2159024E-03	1.7681492E-03	9.9493990E-04
2	0	3	5.1138750E-03	2.6836705E-03	1.4518885E-03
2	0	4	9.0375215E-03	4.4793775E-03	2.3063028E-03
2	1	1	3.1049206E-03	1.7129667E-03	9.6682545E-04
2	1	2	4.7192815E-03	2.4946379E-03	1.3587859E-03
2	1	3	7.8933160E-03	3.9534628E-03	2.0570836E-03
2	1	4	1.4731562E-02	6.9261075E-03	3.4087567E-03
2	2	2	7.5577230E-03	3.7980727E-03	1.9828856E-03
2	2	3	1.3412134E-02	6.3401240E-03	3.1397662E-03
2	2	4	2.6615545E-02	1.1751115E-02	5.4717115E-03
2	3	3	2.5373420E-02	1.1221045E-02	5.2373795E-03
2	3	4	5.3617050E-02	2.2097272E-02	9.6562310E-03
2	4	4	1.2013843E-01	4.6197620E-02	1.8873419E-02

X = 5.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
2	0	0	9.1700010E-03	5.0223505E-03	2.8293935E-03
2	0	1	1.4194038E-02	7.3642065E-03	3.9775219E-03
2	0	2	2.4775924E-02	1.1938927E-02	6.0842540E-03
2	0	3	4.9993845E-02	2.1955684E-02	1.0371132E-02
2	0	4	1.1795748E-01	4.6684000E-02	2.0142412E-02
2	1	1	2.3537755E-02	1.1405692E-02	5.8418665E-03
2	1	2	4.4620226E-02	1.9788662E-02	9.4422665E-03
2	1	3	9.8298875E-02	3.9299869E-02	1.7174816E-02
2	1	4	2.5146516E-01	9.0282240E-02	3.5753945E-02
2	2	2	9.2798800E-02	3.7205279E-02	1.6325759E-02
2	2	3	2.2403297E-01	8.0510150E-02	3.2042945E-02
2	2	4	6.2060580E-01	2.0064246E-01	7.2083660E-02
2	3	3	5.8808440E-01	1.8976548E-01	6.8205390E-02
2	3	4	1.7448625E+00	5.1033285E-01	1.6587087E-01
2	4	4	5.4649255E+00	1.4639907E+00	4.3306460E-01

X = 5.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
2	0	0	1.6280098E-03	9.5228230E-04	5.6439980E-04
2	0	1	2.2132377E-03	1.2598639E-03	7.3006600E-04
2	0	2	3.2324251E-03	1.7725748E-03	9.9619205E-04
2	0	3	5.1800470E-03	2.7013879E-03	1.4568613E-03
2	0	4	9.3134225E-03	4.5532545E-03	2.3269631E-03
2	1	1	3.1177105E-03	1.7163153E-03	9.6772645E-04
2	1	2	4.7626635E-03	2.5057279E-03	1.3617114E-03
2	1	3	8.0570755E-03	3.9948872E-03	2.0679036E-03
2	1	4	1.5389480E-02	7.0917700E-03	3.4518671E-03
2	2	2	7.6933850E-03	3.8313926E-03	1.9913488E-03
2	2	3	1.3893786E-02	6.4557185E-03	3.1684528E-03
2	2	4	2.8469875E-02	1.2190731E-02	5.5795605E-03
2	3	3	2.6995817E-02	1.1596709E-02	5.3272155E-03
2	3	4	5.9616250E-02	2.3456152E-02	9.9740600E-03
2	4	4	1.4158914E-01	5.0908080E-02	1.9939832E-02

X =   5.7

K	M	N	A = 1.0	A = 1.2	A = 1.4
2	0	0	9.1846360E-03	5.0254505E-03	2.8299675E-03
2	0	1	1.4252569E-02	7.3758595E-03	3.9798079E-03
2	0	2	2.5044087E-02	1.1991528E-02	6.0946095E-03
2	0	3	5.1304890E-02	2.2211692E-02	1.0421841E-02
2	0	4	1.2459815E-01	4.7979120E-02	2.0399955E-02
2	1	1	2.3751632E-02	1.1445258E-02	5.8495410E-03
2	1	2	4.5535675E-02	1.9953182E-02	9.4732720E-03
2	1	3	1.0257080E-01	4.0058284E-02	1.7316267E-02
2	1	4	2.7240634E-01	9.3983050E-02	3.6442800E-02
2	2	2	9.6497230E-02	3.7838662E-02	1.6439151E-02
2	2	3	2.4056343E-01	8.3268200E-02	3.2523666E-02
2	2	4	6.9916335E-01	2.1357616E-01	7.4311675E-02
2	3	3	6.5941095E-01	2.0121700E-01	7.0118550E-02
2	3	4	2.0747401E+00	5.6211485E-01	1.7432276E-01
2	4	4	6.9572060E+00	1.6912022E+00	4.6893302E-01

X =   5.7

K	M	N	A = 1.6	A = 1.8	A = 2.0
2	0	0	1.6281314E-03	9.5231665E-04	5.6441400E-04
2	0	1	2.2137231E-03	1.2599775E-03	7.3009835E-04
2	0	2	3.2346201E-03	1.7730799E-03	9.9632240E-04
2	0	3	5.1908460E-03	2.7038403E-03	1.4574603E-03
2	0	4	9.3684405E-03	4.5656900E-03	2.3299279E-03
2	1	1	3.1192759E-03	1.7166410E-03	9.6780020E-04
2	1	2	4.7688030E-03	2.5069904E-03	1.3619874E-03
2	1	3	8.0848435E-03	4.0005610E-03	2.0691237E-03
2	1	4	1.5524455E-02	7.1193725E-03	3.4577893E-03
2	2	2	7.7146695E-03	3.8355784E-03	1.9922144E-03
2	2	3	1.3981667E-02	6.4725360E-03	3.1718245E-03
2	2	4	2.8872503E-02	1.2267006E-02	5.5946945E-03
2	3	3	2.7330137E-02	1.1657695E-02	5.3388395E-03
2	3	4	6.1056360E-02	2.3712255E-02	1.0021617E-02
2	4	4	1.4747341E-01	5.1912830E-02	2.0118514E-02

X =   6.7

K	M	N	A = 1.0	A = 1.2	A = 1.4
2	0	0	9.1904010E-03	5.0262445E-03	2.8301584E-03
2	0	1	1.4279770E-02	7.3800250E-03	3.9805930E-03
2	0	2	2.5186905E-02	1.2013617E-02	6.0985935E-03
2	0	3	5.2111855E-02	2.2338162E-02	1.0444430E-02
2	0	4	1.2931477E-01	4.8724780E-02	2.0532628E-02
2	1	1	2.3862610E-02	1.1461870E-02	5.8521820E-03
2	1	2	4.6068870E-02	2.0030616E-02	9.4852945E-03
2	1	3	1.0541403E-01	4.0466719E-02	1.7379234E-02
2	1	4	2.8844878E-01	9.6281300E-02	3.6796646E-02
2	2	2	9.8873990E-02	3.8163975E-02	1.6486749E-02
2	2	3	2.5255831E-01	8.4859235E-02	3.2749258E-02
2	2	4	7.6430045E-01	2.2209152E-01	7.5502315E-02
2	3	3	7.1727030E-01	2.0851769E-01	7.1098880E-02
2	3	4	2.3783605E+00	5.9936430E-01	1.7917412E-01
2	4	4	8.5067200E+00	1.8738740E+00	4.9166125E-01

X =   6.7

K	M	N	A = 1.6	A = 1.8	A = 2.0
2	0	0	1.6281734E-03	9.5233445E-04	5.6440105E-04
2	0	1	2.2138757E-03	1.2600187E-03	7.3008985E-04
2	0	2	3.2353322E-03	1.7732226E-03	9.9630025E-04
2	0	3	5.1949385E-03	2.7046516E-03	1.4574997E-03
2	0	4	9.3926095E-03	4.5704345E-03	2.3305119E-03
2	1	1	3.1196982E-03	1.7167043E-03	9.6779940E-04
2	1	2	4.7707345E-03	2.5073043E-03	1.3620195E-03
2	1	3	8.0950720E-03	4.0022975E-03	2.0694022E-03
2	1	4	1.5582293E-02	7.1293465E-03	3.4595209E-03
2	2	2	7.7219675E-03	3.8367376E-03	1.9923678E-03
2	2	3	1.4015445E-02	6.4778470E-03	3.1726391E-03
2	2	4	2.9049405E-02	1.2294843E-02	5.5991675E-03
2	3	3	2.7469268E-02	1.1678515E-02	5.3420570E-03
2	3	4	6.1725655E-02	2.3810007E-02	1.0036605E-02
2	4	4	1.5046289E-01	5.2328695E-02	2.0179618E-02

X = 8.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
2	0	0	9.1916690E-03	5.0264385E-03	2.8301640E-03
2	0	1	1.4287548E-02	7.3810740E-03	3.9807179E-03
2	0	2	2.5235995E-02	1.2020040E-02	6.0994025E-03
2	0	3	5.2443395E-02	2.2381476E-02	1.0450121E-02
2	0	4	1.3162431E-01	4.9025920E-02	2.0573033E-02
2	1	1	2.3899051E-02	1.1466216E-02	5.8527580E-03
2	1	2	4.6268560E-02	2.0053248E-02	9.4881075E-03
2	1	3	1.0665668E-01	4.0605783E-02	1.7396261E-02
2	1	4	2.9671435E-01	9.7201345E-02	3.6909085E-02
2	2	2	9.9860200E-02	3.8266631E-02	1.6498409E-02
2	2	3	2.5825388E-01	8.5429685E-02	3.2811574E-02
2	2	4	8.0034880E-01	2.2563493E-01	7.5884405E-02
2	3	3	7.4816120E-01	2.1141277E-01	7.1393320E-02
2	3	4	2.5649015E+00	6.1618625E-01	1.8082382E-01
2	4	4	9.5904020E+00	1.9662367E+00	5.0019390E-01

X = 8.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
2	0	0	1.6281899E-03	9.5231020E-04	5.6440635E-04
2	0	1	2.2139145E-03	1.2599955E-03	7.3009535E-04
2	0	2	3.2355019E-03	1.7731749E-03	9.9631540E-04
2	0	3	5.1959400E-03	2.7045936E-03	1.4575518E-03
2	0	4	9.3991855E-03	4.5707360E-03	2.3307550E-03
2	1	1	3.1197904E-03	1.7167120E-03	9.6780060E-04
2	1	2	4.7711305E-03	2.5073448E-03	1.3620281E-03
2	1	3	8.0973765E-03	4.0025855E-03	2.0694482E-03
2	1	4	1.5597308E-02	7.1313730E-03	3.4598233E-03
2	2	2	7.7234310E-03	3.8368921E-03	1.9924001E-03
2	2	3	1.4022910E-02	6.4787135E-03	3.1727773E-03
2	2	4	2.9094465E-02	1.2300354E-02	5.5999595E-03
2	3	3	2.7501949E-02	1.1682234E-02	5.3425620E-03
2	3	4	6.1901845E-02	2.3830010E-02	1.0039130E-02
2	4	4	1.5131693E-01	5.2420985E-02	2.0190332E-02

X = 10.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
2	0	0	9.1924070E-03	5.0265500E-03	2.8301908E-03
2	0	1	1.4290081E-02	7.3813725E-03	3.9807600E-03
2	0	2	2.5252392E-02	1.2021727E-02	6.0996130E-03
2	0	3	5.2566255E-02	2.2393279E-02	1.0451388E-02
2	0	4	1.3262490E-01	4.9120460E-02	2.0583092E-02
2	1	1	2.3907641E-02	1.1466976E-02	5.8528100E-03
2	1	2	4.6322150E-02	2.0057569E-02	9.4884060E-03
2	1	3	1.0705469E-01	4.0637666E-02	1.7398819E-02
2	1	4	2.9991589E-01	9.7459425E-02	3.6931554E-02
2	2	2	1.0015200E-01	3.8287944E-02	1.6499963E-02
2	2	3	2.6020191E-01	8.5565795E-02	3.2821686E-02
2	2	4	8.1500860E-01	2.2664751E-01	7.5962305E-02
2	3	3	7.6000550E-01	2.1217054E-01	7.1445995E-02
2	3	4	2.6481072E+00	6.2128925E-01	1.8117364E-01
2	4	4	1.0141627E+01	1.9976408E+00	5.0221105E-01

X = 10.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
2	0	0	1.6281848E-03	9.5233530E-04	5.6441040E-04
2	0	1	2.2139076E-03	1.2600220E-03	7.3010000E-04
2	0	2	3.2355003E-03	1.7732439E-03	9.9632540E-04
2	0	3	5.1959590E-03	2.7047751E-03	1.4575625E-03
2	0	4	9.3998685E-03	4.5714315E-03	2.3308112E-03
2	1	1	3.1197828E-03	1.7167164E-03	9.6780310E-04
2	1	2	4.7711035E-03	2.5073333E-03	1.3620160E-03
2	1	3	8.0974810E-03	4.0025846E-03	2.0694277E-03
2	1	4	1.5599089E-02	7.1315290E-03	3.4598041E-03
2	2	2	7.7234720E-03	3.8368788E-03	1.9923744E-03
2	2	3	1.4023580E-02	6.4787610E-03	3.1727384E-03
2	2	4	2.9100661E-02	1.2300859E-02	5.5999100E-03
2	3	3	2.7505745E-02	1.1682577E-02	5.3425105E-03
2	3	4	6.1928000E-02	2.3832166E-02	1.0039153E-02
2	4	4	1.5146024E-01	5.2431660E-02	2.0190963E-02

X = 15.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
2	0	0	9.1919070E-03	5.0265330E-03	2.8301143E-03
2	0	1	1.4289418E-02	7.3813605E-03	3.9806714E-03
2	0	2	2.5250539E-02	1.2021768E-02	6.0993380E-03
2	0	3	5.2565350E-02	2.2393955E-02	1.0450457E-02
2	0	4	1.3269513E-01	4.9129415E-02	2.0579356E-02
2	1	1	2.3908601E-02	1.1467037E-02	5.8528370E-03
2	1	2	4.6329015E-02	2.0057974E-02	9.4884815E-03
2	1	3	1.0711501E-01	4.0640597E-02	1.7399188E-02
2	1	4	3.0053061E-01	9.7490590E-02	3.6934059E-02
2	2	2	1.0019004E-01	3.8289817E-02	1.6500075E-02
2	2	3	2.6050175E-01	8.5578615E-02	3.2822491E-02
2	2	4	8.1782670E-01	2.2676905E-01	7.5968605E-02
2	3	3	7.6203955E-01	2.1224534E-01	7.1450450E-02
2	3	4	2.6652131E+00	6.2190380E-01	1.8120321E-01
2	4	4	1.0271350E+01	2.0018997E+00	5.0238310E-01

X = 15.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
2	0	0	1.6281540E-03	9.5231780E-04	5.6439815E-04
2	0	1	2.2138730E-03	1.2600039E-03	7.3008850E-04
2	0	2	3.2354072E-03	1.7731993E-03	9.9629770E-04
2	0	3	5.1956630E-03	2.7046443E-03	1.4574901E-03
2	0	4	9.3987530E-03	4.5709810E-03	2.3305777E-03
2	1	1	3.1197845E-03	1.7167163E-03	9.6780390E-04
2	1	2	4.7711095E-03	2.5073346E-03	1.3620150E-03
2	1	3	8.0974580E-03	4.0025544E-03	2.0694098E-03
2	1	4	1.5599159E-02	7.1314905E-03	3.4597767E-03
2	2	2	7.7234370E-03	3.8368555E-03	1.9923476E-03
2	2	3	1.4023470E-02	6.4786785E-03	3.1726776E-03
2	2	4	2.9100701E-02	1.2300745E-02	5.5997890E-03
2	3	3	2.7505443E-02	1.1682304E-02	5.3423800E-03
2	3	4	6.1928260E-02	2.3831686E-02	1.0038903E-02
2	4	4	1.5146665E-01	5.2431550E-02	2.0190668E-02

X = 20.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
2	0	0	9.1940980E-03	5.0273335E-03	2.8305458E-03
2	0	1	1.4292871E-02	7.3824165E-03	3.9811840E-03
2	0	2	2.5264976E-02	1.2025509E-02	6.1009230E-03
2	0	3	5.2638500E-02	2.2409880E-02	1.0456242E-02
2	0	4	1.3313206E-01	4.9208410E-02	2.0603925E-02
2	1	1	2.3907959E-02	1.1466767E-02	5.8527455E-03
2	1	2	4.6326985E-02	2.0057209E-02	9.4882665E-03
2	1	3	1.0710556E-01	4.0637619E-02	1.7398401E-02
2	1	4	3.0047005E-01	9.7474630E-02	3.6930137E-02
2	2	2	1.0018499E-01	3.8287947E-02	1.6499688E-02
2	2	3	2.6049112E-01	8.5574495E-02	3.2821925E-02
2	2	4	8.1774505E-01	2.2674414E-01	7.5964295E-02
2	3	3	7.6205905E-01	2.1224344E-01	7.1451260E-02
2	3	4	2.6652336E+00	6.2187435E-01	1.8119920E-01
2	4	4	1.0270884E+01	2.0016505E+00	5.0233295E-01

X = 20.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
2	0	0	1.6283487E-03	9.5240035E-04	5.6444535E-04
2	0	1	2.2140850E-03	1.2600848E-03	7.3013045E-04
2	0	2	3.2359854E-03	1.7734003E-03	9.9639640E-04
2	0	3	5.1975290E-03	2.7052297E-03	1.4577504E-03
2	0	4	9.4056730E-03	4.5729015E-03	2.3313527E-03
2	1	1	3.1197636E-03	1.7167037E-03	9.6779495E-04
2	1	2	4.7710600E-03	2.5073064E-03	1.3620014E-03
2	1	3	8.0972880E-03	4.0024796E-03	2.0693704E-03
2	1	4	1.5598333E-02	7.1311730E-03	3.4596370E-03
2	2	2	7.7233340E-03	3.8368005E-03	1.9923332E-03
2	2	3	1.4023385E-02	6.4786330E-03	3.1726707E-03
2	2	4	2.9099795E-02	1.2300392E-02	5.5997085E-03
2	3	3	2.7505879E-02	1.1682467E-02	5.3424300E-03
2	3	4	6.1927815E-02	2.3831578E-02	1.0038866E-02
2	4	4	1.5145681E-01	5.2428915E-02	2.0189943E-02

X = 30.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
2	0	0	9.1912360E-03	5.0262205E-03	2.8300687E-03
2	0	1	1.4288346E-02	7.3809175E-03	3.9806131E-03
2	0	2	2.5246150E-02	1.2020245E-02	6.0991625E-03
2	0	3	5.2542890E-02	2.2387592E-02	1.0449801E-02
2	0	4	1.3255960E-01	4.9097480E-02	2.0576717E-02
2	1	1	2.3908725E-02	1.1467040E-02	5.8528250E-03
2	1	2	4.6329330E-02	2.0058006E-02	9.4884505E-03
2	1	3	1.0711326E-01	4.0640908E-02	1.7399065E-02
2	1	4	3.0042924E-01	9.7492255E-02	3.6934054E-02
2	2	2	1.0018790E-01	3.8289864E-02	1.6500012E-02
2	2	3	2.6038586E-01	8.5579045E-02	3.2822239E-02
2	2	4	8.1406380E-01	2.2676638E-01	7.5969175E-02
2	3	3	7.5822865E-01	2.1224293E-01	7.1449510E-02
2	3	4	2.6447678E+00	6.2189510E-01	1.8120402E-01
2	4	4	1.0164016E+01	2.0018752E+00	5.0240810E-01

X = 30.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
2	0	0	1.6281455E-03	9.5230915E-04	5.6439245E-04
2	0	1	2.2138697E-03	1.2599961E-03	7.3008225E-04
2	0	2	3.2353938E-03	1.7731786E-03	9.9628460E-04
2	0	3	5.1956155E-03	2.7045831E-03	1.4574540E-03
2	0	4	9.3986240E-03	4.5707910E-03	2.3304878E-03
2	1	1	3.1198043E-03	1.7167192E-03	9.6780200E-04
2	1	2	4.7711485E-03	2.5073362E-03	1.3620122E-03
2	1	3	8.0975745E-03	4.0025582E-03	2.0693997E-03
2	1	4	1.5599700E-02	7.1315215E-03	3.4597682E-03
2	2	2	7.7234975E-03	3.8368449E-03	1.9923445E-03
2	2	3	1.4023624E-02	6.4786235E-03	3.1726434E-03
2	2	4	2.9101607E-02	1.2300672E-02	5.5997655E-03
2	3	3	2.7505849E-02	1.1682140E-02	5.3422505E-03
2	3	4	6.1930600E-02	2.3831561E-02	1.0038788E-02
2	4	4	1.5147855E-01	5.2432570E-02	2.0191168E-02

X = 40.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
2	0	0	9.1912360E-03	5.0262205E-03	2.8300687E-03
2	0	1	1.4288346E-02	7.3809175E-03	3.9806131E-03
2	0	2	2.5246150E-02	1.2020247E-02	6.0991625E-03
2	0	3	5.2542985E-02	2.2387600E-02	1.0449801E-02
2	0	4	1.3256323E-01	4.9097510E-02	2.0576717E-02
2	1	1	2.3908725E-02	1.1467042E-02	5.8528250E-03
2	1	2	4.6329425E-02	2.0058013E-02	9.4884505E-03
2	1	3	1.0711687E-01	4.0640930E-02	1.7399065E-02
2	1	4	3.0054862E-01	9.7492440E-02	3.6934054E-02
2	2	2	1.0019153E-01	3.8289887E-02	1.6500012E-02
2	2	3	2.6050500E-01	8.5579210E-02	3.2822239E-02
2	2	4	8.1787520E-01	2.2677227E-01	7.5969175E-02
2	3	3	7.6203505E-01	2.1224875E-01	7.1449510E-02
2	3	4	2.6653415E+00	6.2192140E-01	1.8120402E-01
2	4	4	1.0273062E+01	2.0019907E+00	5.0240810E-01

X = 40.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
2	0	0	1.6281458E-03	9.5230915E-04	5.6439245E-04
2	0	1	2.2138701E-03	1.2599961E-03	7.3008225E-04
2	0	2	3.2353945E-03	1.7731786E-03	9.9628460E-04
2	0	3	5.1956175E-03	2.7045831E-03	1.4574540E-03
2	0	4	9.3986315E-03	4.5707910E-03	2.3304878E-03
2	1	1	3.1198049E-03	1.7167192E-03	9.6780200E-04
2	1	2	4.7711485E-03	2.5073362E-03	1.3620122E-03
2	1	3	8.0975775E-03	4.0025582E-03	2.0693997E-03
2	1	4	1.5599711E-02	7.1315215E-03	3.4597682E-03
2	2	2	7.7234975E-03	3.8368449E-03	1.9923445E-03
2	2	3	1.4023624E-02	6.4786235E-03	3.1726434E-03
2	2	4	2.9101607E-02	1.2300672E-02	5.5997655E-03
2	3	3	2.7505849E-02	1.1682140E-02	5.3422505E-03
2	3	4	6.1930600E-02	2.3831561E-02	1.0038788E-02
2	4	4	1.5147856E-01	5.2432570E-02	2.0191166E-02

X = ∞

K	M	N	A = 1.0	A = 1.2	A = 1.4
2	0	0	9.1912360E-03	5.0262205E-03	2.8300687E-03
2	0	1	1.4288346E-02	7.3809175E-03	3.9806131E-03
2	0	2	2.5246150E-02	1.2020247E-02	6.0991625E-03
2	0	3	5.2542985E-02	2.2387600E-02	1.0449801E-02
2	0	4	1.3256323E-01	4.9097510E-02	2.0576717E-02
2	1	1	2.3908725E-02	1.1467042E-02	5.8528250E-03
2	1	2	4.6329425E-02	2.0058013E-02	9.4884505E-03
2	1	3	1.0711687E-01	4.0640930E-02	1.7399065E-02
2	1	4	3.0054862E-01	9.7492440E-02	3.6934054E-02
2	2	2	1.0019153E-01	3.8289887E-02	1.6500012E-02
2	2	3	2.6050500E-01	8.5579210E-02	3.2822239E-02
2	2	4	8.1787520E-01	2.2677227E-01	7.5969175E-02
2	3	3	7.6203505E-01	2.1224875E-01	7.1449510E-02
2	3	4	2.66653415E+00	6.2192140E-01	1.8120402E-01
2	4	4	1.0273062E+01	2.0019907E+00	5.0240810E-01

X = ∞

K	M	N	A = 1.6	A = 1.8	A = 2.0
2	0	0	1.6281458E-03	9.5230915E-04	5.6439245E-04
2	0	1	2.2138701E-03	1.2599961E-03	7.3008225E-04
2	0	2	3.2353945E-03	1.7731786E-03	9.9628460E-04
2	0	3	5.1956175E-03	2.7045831E-03	1.4574540E-03
2	0	4	9.3986315E-03	4.5707910E-03	2.3304878E-03
2	1	1	3.1198049E-03	1.7167192E-03	9.6780200E-04
2	1	2	4.7711485E-03	2.5073362E-03	1.3620122E-03
2	1	3	8.0975775E-03	4.0025582E-03	2.0693997E-03
2	1	4	1.5599711E-02	7.1315215E-03	3.4597682E-03
2	2	2	7.7234975E-03	3.8368449E-03	1.9923445E-03
2	2	3	1.4023624E-02	6.4786235E-03	3.1726434E-03
2	2	4	2.91011607E-02	1.2300672E-02	5.5997655E-03
2	3	3	2.7505849E-02	1.1682140E-02	5.3422505E-03
2	3	4	6.1930600E-02	2.3831561E-02	1.0038788E-02
2	4	4	1.5147856E-01	5.2432570E-02	2.0191166E-02

X =   4.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
3	0	0	5.0037640E-03	2.7722582E-03	1.5760452E-03
3	0	1	7.5793070E-03	3.9954550E-03	2.1827089E-03
3	0	2	1.2724892E-02	6.2895520E-03	3.2591855E-03
3	0	3	2.4064481E-02	1.1016321E-02	5.3446710E-03
3	0	4	5.1517555E-02	2.1724253E-02	9.7769495E-03
3	1	1	1.2339173E-02	6.1138910E-03	3.1760745E-03
3	1	2	2.2509898E-02	1.0343235E-02	5.0407295E-03
3	1	3	4.6390070E-02	1.9616583E-02	8.8706140E-03
3	1	4	1.0749176E-01	4.1866885E-02	1.7484836E-02
3	2	2	4.4850765E-02	1.8981553E-02	8.5966940E-03
3	2	3	1.0050708E-01	3.9126895E-02	1.6360040E-02
3	2	4	2.5017229E-01	9.0170490E-02	3.4839256E-02
3	3	3	2.4239110E-01	8.7263130E-02	3.3704568E-02
3	3	4	6.4011470E-01	2.1521168E-01	7.7217960E-02
3	4	4	1.7703180E+00	5.6110080E-01	1.8850225E-01

X =   4.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
3	0	0	9.1399405E-04	5.3842410E-04	3.2119100E-04
3	0	1	1.2256993E-03	7.0325935E-04	4.1043810E-04
3	0	2	1.7529430E-03	9.7086170E-04	5.5030335E-04
3	0	3	2.7196070E-03	1.4383280E-03	7.8454225E-04
3	0	4	4.6547960E-03	2.3247696E-03	1.2076787E-03
3	1	1	1.7123255E-03	9.5040635E-04	5.3974825E-04
3	1	2	2.5773874E-03	1.3694646E-03	7.5022985E-04
3	1	3	4.2503060E-03	2.1372493E-03	1.1179307E-03
3	1	4	7.8848980E-03	3.6673805E-03	1.8127687E-03
3	2	2	4.1275060E-03	2.0801242E-03	1.0904363E-03
3	2	3	7.3043020E-03	3.4537755E-03	1.7142491E-03
3	2	4	1.4405832E-02	6.3435230E-03	2.9539918E-03
3	3	3	1.3942777E-02	6.1466430E-03	2.8670149E-03
3	3	4	2.9621169E-02	1.2132448E-02	5.2833800E-03
3	4	4	6.7400285E-02	2.5694436E-02	1.0431717E-02

X =   5.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
3	0	0	5.0350560E-03	2.7796678E-03	1.5778552E-03
3	0	1	7.6935315E-03	4.0218360E-03	2.1890047E-03
3	0	2	1.3170570E-02	6.3911215E-03	3.2831210E-03
3	0	3	2.5878017E-02	1.1426531E-02	5.4406325E-03
3	0	4	5.9099900E-02	2.3431664E-02	1.0174522E-02
3	1	1	1.2740922E-02	6.2034235E-03	3.1966910E-03
3	1	2	2.4033879E-02	1.0675526E-02	5.1155875E-03
3	1	3	5.2464955E-02	2.0923121E-02	9.1609650E-03
3	1	4	1.3251858E-01	4.7199295E-02	1.8659858E-02
3	2	2	5.0501715E-02	2.0178473E-02	8.8582305E-03
3	2	3	1.2264259E-01	4.3725880E-02	1.7344734E-02
3	2	4	3.4016538E-01	1.0861689E-01	3.8736962E-02
3	3	3	3.2790819E-01	1.0461033E-01	3.7322428E-02
3	3	4	9.8408970E-01	2.8379665E-01	9.1267185E-02
3	4	4	3.1421372E+00	8.2912010E-01	2.4221966E-01

X =   5.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
3	0	0	9.1445080E-04	5.3854140E-04	3.2122330E-04
3	0	1	1.2272537E-03	7.0365375E-04	4.1054275E-04
3	0	2	1.7587806E-03	9.7232675E-04	5.5068735E-04
3	0	3	2.7428761E-03	1.4441493E-03	7.8606100E-04
3	0	4	4.7508850E-03	2.3487514E-03	1.2139243E-03
3	1	1	1.7172352E-03	9.5161340E-04	5.4005420E-04
3	1	2	2.5948093E-03	1.3736479E-03	7.5126635E-04
3	1	3	4.3170230E-03	2.1530915E-03	1.1218129E-03
3	1	4	8.0528990E-03	3.7305935E-03	1.8281784E-03
3	2	2	4.1863945E-03	2.0937819E-03	1.0937033E-03
3	2	3	7.5214910E-03	3.5031445E-03	1.7258152E-03
3	2	4	1.5254348E-02	6.5339420E-03	2.9980862E-03
3	3	3	1.4719005E-02	6.3181430E-03	2.9059872E-03
3	3	4	3.2579964E-02	1.2773663E-02	5.4263135E-03
3	4	4	7.8452325E-02	2.8030231E-02	1.0938996E-02

X =   5.7

K	M	N	A = 1.0	A = 1.2	A = 1.4
3	0	0	5.0403230E-03	2.7806303E-03	1.5780336E-03
3	0	1	7.7161275E-03	4.0258770E-03	2.1897499E-03
3	0	2	1.3275927E-02	6.4096840E-03	3.2865250E-03
3	0	3	2.6392883E-02	1.1516830E-02	5.4571710E-03
3	0	4	6.1688415E-02	2.3884941E-02	1.0257593E-02
3	1	1	1.2832720E-02	6.2191810E-03	3.1994970E-03
3	1	2	2.4444700E-02	1.0744135E-02	5.1275040E-03
3	1	3	5.4413360E-02	2.1244460E-02	9.2160975E-03
3	1	4	1.4210171E-01	4.8771235E-02	1.8928130E-02
3	2	2	5.2279740E-02	2.0463975E-02	8.9059035E-03
3	2	3	1.3085931E-01	4.5017025E-02	1.7555463E-02
3	2	4	3.7979573E-01	1.1476841E-01	3.9728728E-02
3	3	3	3.6507331E-01	1.1028304E-01	3.8218749E-02
3	3	4	1.1603014E+00	3.1021301E-01	9.5360195E-02
3	4	4	3.9659955E+00	9.4983785E-01	2.6044626E-01

X =   5.7

K	M	N	A = 1.6	A = 1.8	A = 2.0
3	0	0	9.1448905E-04	5.3855020E-04	3.2122525E-04
3	0	1	1.2274028E-03	7.0368520E-04	4.1054935E-04
3	0	2	1.7594533E-03	9.7246695E-04	5.5071735E-04
3	0	3	2.7461407E-03	1.4448223E-03	7.8620275E-04
3	0	4	4.7672905E-03	2.3521253E-03	1.2146350E-03
3	1	1	1.7177550E-03	9.5171535E-04	5.4007400E-04
3	1	2	2.5969663E-03	1.3740613E-03	7.5134845E-04
3	1	3	4.3269210E-03	2.1549603E-03	1.1221776E-03
3	1	4	8.1008735E-03	3.7396215E-03	1.8299373E-03
3	2	2	4.1946765E-03	2.0952998E-03	1.0939987E-03
3	2	3	7.5573070E-03	3.5095225E-03	1.7270097E-03
3	2	4	1.5420852E-02	6.5632335E-03	3.0034894E-03
3	3	3	1.4866212E-02	6.3432805E-03	2.9104680E-03
3	3	4	3.3237874E-02	1.2883480E-02	5.4453995E-03
3	4	4	8.1296560E-02	2.8489707E-02	1.1015978E-02

X = 6.7

K	M	N	A = 1.0	A = 1.2	A = 1.4
3	0	0	5.0423980E-03	2.7809410E-03	1.5780847E-03
3	0	1	7.7261465E-03	4.0273160E-03	2.1899751E-03
3	0	2	1.3328964E-02	6.4172965E-03	3.2877005E-03
3	0	3	2.6690794E-02	1.1559378E-02	5.4637360E-03
3	0	4	6.3415020E-02	2.4131376E-02	1.0295593E-02
3	1	1	1.2877764E-02	6.2252470E-03	3.2003805E-03
3	1	2	2.4671018E-02	1.0774001E-02	5.1317240E-03
3	1	3	5.5639080E-02	2.1403594E-02	9.2383485E-03
3	1	4	1.4903051E-01	4.9663670E-02	1.9052265E-02
3	2	2	5.3368560E-02	2.0602177E-02	8.9244275E-03
3	2	3	1.3656199E-01	4.5720310E-02	1.7647203E-02
3	2	4	4.1121679E-01	1.1858509E-01	4.0218810E-02
3	3	3	3.9414734E-01	1.1372789E-01	3.8649744E-02
3	3	4	1.3171492E+00	3.2835973E-01	9.7570995E-02
3	4	4	4.7975605E+00	1.0431094E+00	2.7140560E-01

X = 6.7

K	M	N	A = 1.6	A = 1.8	A = 2.0
3	0	0	9.1450040E-04	5.3855060E-04	3.2122535E-04
3	0	1	1.2274434E-03	7.0369055E-04	4.1055055E-04
3	0	2	1.7596612E-03	9.7249580E-04	5.5072275E-04
3	0	3	2.7472614E-03	1.4449925E-03	7.8623480E-04
3	0	4	4.7737185E-03	2.3531425E-03	1.2148269E-03
3	1	1	1.7178901E-03	9.5173900E-04	5.4007875E-04
3	1	2	2.5976066E-03	1.3741633E-03	7.5136620E-04
3	1	3	4.3302205E-03	2.1554868E-03	1.1222680E-03
3	1	4	8.1192450E-03	3.7425470E-03	1.8304380E-03
3	2	2	4.1973665E-03	2.0956922E-03	1.0940598E-03
3	2	3	7.5700870E-03	3.5113650E-03	1.7272916E-03
3	2	4	1.5488123E-02	6.5728590E-03	3.0049634E-03
3	3	3	1.4923013E-02	6.3511580E-03	2.9116189E-03
3	3	4	3.3521506E-02	1.2921827E-02	5.4508940E-03
3	4	4	8.2648710E-02	2.8665161E-02	1.1040127E-02

X = 8.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
3	0	0	5.0429030E-03	2.7809866E-03	1.5780978E-03
3	0	1	7.7288410E-03	4.0276075E-03	2.1900227E-03
3	0	2	1.3345812E-02	6.4190715E-03	3.2879615E-03
3	0	3	2.6802187E-02	1.1571191E-02	5.4653650E-03
3	0	4	6.4177805E-02	2.4212659E-02	1.0306516E-02
3	1	1	1.2890900E-02	6.2267045E-03	3.2005470E-03
3	1	2	2.4747614E-02	1.0781883E-02	5.1325915E-03
3	1	3	5.6122215E-02	2.1452256E-02	9.2435770E-03
3	1	4	1.5223233E-01	4.9983655E-02	1.9086548E-02
3	2	2	5.3788065E-02	2.0641658E-02	8.9284930E-03
3	2	3	1.3908964E-01	4.5949555E-02	1.7669805E-02
3	2	4	4.2743619E-01	1.2002874E-01	4.0358975E-02
3	3	3	4.0881606E-01	1.1498801E-01	3.8766400E-02
3	3	4	1.4085792E+00	3.3596653E-01	9.8253450E-02
3	4	4	5.3539180E+00	1.0874248E+00	2.7519852E-01

X = 8.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
3	0	0	9.1450005E-04	5.3855175E-04	3.2122585E-04
3	0	1	1.2274462E-03	7.0369225E-04	4.1055130E-04
3	0	2	1.7596826E-03	9.7250470E-04	5.5072520E-04
3	0	3	2.7474326E-03	1.4450313E-03	7.8624315E-04
3	0	4	4.7749505E-03	2.3533796E-03	1.2148703E-03
3	1	1	1.7179078E-03	9.5174090E-04	5.4007985E-04
3	1	2	2.5976985E-03	1.3741786E-03	7.5136925E-04
3	1	3	4.3308165E-03	2.1555593E-03	1.1222799E-03
3	1	4	8.1231720E-03	3.7430425E-03	1.8305138E-03
3	2	2	4.1977750E-03	2.0957644E-03	1.0940683E-03
3	2	3	7.5724245E-03	3.5116715E-03	1.7273267E-03
3	2	4	1.5502520E-02	6.5746830E-03	3.0051787E-03
3	3	3	1.4934766E-02	6.3524010E-03	2.9117551E-03
3	3	4	3.3587877E-02	1.2928775E-02	5.4516565E-03
3	4	4	8.2998105E-02	2.8700204E-02	1.1043817E-02

X = 10.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
3	0	0	5.0429720E-03	2.7810005E-03	1.5780884E-03
3	0	1	7.7293285E-03	4.0276570E-03	2.1900084E-03
3	0	2	1.3349397E-02	6.4194250E-03	3.2879300E-03
3	0	3	2.6831024E-02	1.1573862E-02	5.4653270E-03
3	0	4	6.4417705E-02	2.4234120E-02	1.0307024E-02
3	1	1	1.2893728E-02	6.2268675E-03	3.2005505E-03
3	1	2	2.4766121E-02	1.0783091E-02	5.1326715E-03
3	1	3	5.6260350E-02	2.1461377E-02	9.2442280E-03
3	1	4	1.5333147E-01	5.0056755E-02	1.9091992E-02
3	2	2	5.3899465E-02	2.0648883E-02	8.9290355E-03
3	2	3	1.3986919E-01	4.5998000E-02	1.7673254E-02
3	2	4	4.3336786E-01	1.2038953E-01	4.0384130E-02
3	3	3	4.1397000E-01	1.1528602E-01	3.8785922E-02
3	3	4	1.4461317E+00	3.3804631E-01	9.8383840E-02
3	4	4	5.6178090E+00	1.1011512E+00	2.7600222E-01

X = 10.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
3	0	0	9.1450070E-04	5.3855150E-04	3.2122545E-04
3	0	1	1.2274474E-03	7.0369030E-04	4.1055080E-04
3	0	2	1.7596872E-03	9.7250165E-04	5.5072315E-04
3	0	3	2.7474606E-03	1.4450295E-03	7.8623930E-04
3	0	4	4.7751630E-03	2.3533794E-03	1.2148585E-03
3	1	1	1.7179107E-03	9.5173305E-04	5.4008020E-04
3	1	2	2.5977093E-03	1.3741624E-03	7.5136850E-04
3	1	3	4.3308875E-03	2.1555256E-03	1.1222819E-03
3	1	4	8.1237350E-03	3.7429265E-03	1.8305263E-03
3	2	2	4.1978175E-03	2.0957387E-03	1.0940604E-03
3	2	3	7.5726855E-03	3.5116475E-03	1.7273138E-03
3	2	4	1.5504476E-02	6.5746385E-03	3.0051474E-03
3	3	3	1.4936122E-02	6.3525415E-03	2.9117526E-03
3	3	4	3.3596881E-02	1.2929500E-02	5.4516935E-03
3	4	4	8.3050835E-02	2.8703736E-02	1.1044112E-02

X = 15.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
3	0	0	5.0429720E-03	2.7810145E-03	1.5780986E-03
3	0	1	7.7293655E-03	4.0276820E-03	2.1900260E-03
3	0	2	1.3349725E-02	6.4195420E-03	3.2879865E-03
3	0	3	2.6834217E-02	1.1574584E-02	5.4655965E-03
3	0	4	6.4452445E-02	2.4239191E-02	1.0308454E-02
3	1	1	1.2894033E-02	6.2268675E-03	3.2005575E-03
3	1	2	2.4768244E-02	1.0783120E-02	5.1326735E-03
3	1	3	5.6278135E-02	2.1461989E-02	9.2443105E-03
3	1	4	1.5350636E-01	5.0063275E-02	1.9092601E-02
3	2	2	5.3913055E-02	2.0649138E-02	8.9289615E-03
3	2	3	1.3997495E-01	4.6001305E-02	1.7673197E-02
3	2	4	4.3434953E-01	1.2042122E-01	4.0384575E-02
3	3	3	4.1473638E-01	1.1531271E-01	3.8786838E-02
3	3	4	1.4528074E+00	3.3826338E-01	9.8391650E-02
3	4	4	5.6723325E+00	1.1027584E+00	2.7605750E-01

X = 15.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
3	0	0	9.1450125E-04	5.3855190E-04	3.2122535E-04
3	0	1	1.2274481E-03	7.0369235E-04	4.1055055E-04
3	0	2	1.7596918E-03	9.7250445E-04	5.5072410E-04
3	0	3	2.7474760E-03	1.4450346E-03	7.8623840E-04
3	0	4	4.7752320E-03	2.3533992E-03	1.2148549E-03
3	1	1	1.7179091E-03	9.5174100E-04	5.4007875E-04
3	1	2	2.5977103E-03	1.3741779E-03	7.5136905E-04
3	1	3	4.3308830E-03	2.1555666E-03	1.1222756E-03
3	1	4	8.1237140E-03	3.7430890E-03	1.8305020E-03
3	2	2	4.1978375E-03	2.0957594E-03	1.0940753E-03
3	2	3	7.5727375E-03	3.5116825E-03	1.7273382E-03
3	2	4	1.5504712E-02	6.5747770E-03	3.0052304E-03
3	3	3	1.4936231E-02	6.3525370E-03	2.9117585E-03
3	3	4	3.3597399E-02	1.2929485E-02	5.4517020E-03
3	4	4	8.3053285E-02	2.8703684E-02	1.1044100E-02

X = 20.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
3	0	0	5.0429770E-03	2.7809980E-03	1.5780968E-03
3	0	1	7.7293830E-03	4.0276510E-03	2.1900281E-03
3	0	2	1.3349792E-02	6.4194235E-03	3.2879845E-03
3	0	3	2.6834557E-02	1.1573935E-02	5.4655630E-03
3	0	4	6.4454880E-02	2.4235334E-02	1.0308283E-02
3	1	1	1.2894095E-02	6.2268715E-03	3.2005845E-03
3	1	2	2.4768479E-02	1.0783174E-02	5.1327410E-03
3	1	3	5.6279235E-02	2.1462066E-02	9.2445340E-03
3	1	4	1.5351425E-01	5.0063575E-02	1.9093726E-02
3	2	2	5.3913795E-02	2.0649518E-02	8.9290825E-03
3	2	3	1.3997775E-01	4.6002380E-02	1.7673461E-02
3	2	4	4.3436999E-01	1.2042680E-01	4.0385900E-02
3	3	3	4.1474319E-01	1.1531379E-01	3.8786843E-02
3	3	4	1.4528594E+00	3.3826608E-01	9.8391605E-02
3	4	4	5.6727250E+00	1.1027527E+00	2.7605685E-01

X = 20.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
3	0	0	9.1449870E-04	5.3855115E-04	3.2122500E-04
3	0	1	1.2274448E-03	7.0369135E-04	4.1055045E-04
3	0	2	1.7596783E-03	9.7250235E-04	5.5072190E-04
3	0	3	2.7474264E-03	1.4450265E-03	7.8623435E-04
3	0	4	4.7750140E-03	2.3533660E-03	1.2148425E-03
3	1	1	1.7179125E-03	9.5174025E-04	5.4008070E-04
3	1	2	2.5977134E-03	1.3741770E-03	7.5136920E-04
3	1	3	4.3309010E-03	2.1555637E-03	1.1222831E-03
3	1	4	8.1238015E-03	3.7430730E-03	1.8305328E-03
3	2	2	4.1978220E-03	2.0957628E-03	1.0940620E-03
3	2	3	7.5726960E-03	3.5116930E-03	1.7273145E-03
3	2	4	1.5504556E-02	6.5748050E-03	3.0051545E-03
3	3	3	1.4936142E-02	6.3525695E-03	2.9117399E-03
3	3	4	3.3597117E-02	1.2929564E-02	5.4516655E-03
3	4	4	8.3052515E-02	2.8703810E-02	1.1044074E-02

X = 30.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
3	0	0	5.0429770E-03	2.7810093E-03	1.5780970E-03
3	0	1	7.7293880E-03	4.0276765E-03	2.1900273E-03
3	0	2	1.3349807E-02	6.4195025E-03	3.2879825E-03
3	0	3	2.6834617E-02	1.1574377E-02	5.4655555E-03
3	0	4	6.4455295E-02	2.4238001E-02	1.0308245E-02
3	1	1	1.2894110E-02	6.2268945E-03	3.2005825E-03
3	1	2	2.4768529E-02	1.0783182E-02	5.1327360E-03
3	1	3	5.6279450E-02	2.1462273E-02	9.2445135E-03
3	1	4	1.5351577E-01	5.0065015E-02	1.9093633E-02
3	2	2	5.3913955E-02	2.0649158E-02	8.9290730E-03
3	2	3	1.3997831E-01	4.6001265E-02	1.7673425E-02
3	2	4	4.3437392E-01	1.2042130E-01	4.0385735E-02
3	3	3	4.1474402E-01	1.1531175E-01	3.8786697E-02
3	3	4	1.4528657E+00	3.3825940E-01	9.8390950E-02
3	4	4	5.6727735E+00	1.1027448E+00	2.7605391E-01

X = 30.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
3	0	0	9.1449855E-04	5.3855030E-04	3.2122525E-04
3	0	1	1.2274432E-03	7.0369000E-04	4.1055085E-04
3	0	2	1.7596788E-03	9.7249840E-04	5.5072265E-04
3	0	3	2.7474262E-03	1.4450181E-03	7.8623625E-04
3	0	4	4.7750095E-03	2.3533348E-03	1.2148484E-03
3	1	1	1.7179041E-03	9.5173805E-04	5.4008105E-04
3	1	2	2.5977008E-03	1.3741694E-03	7.5137020E-04
3	1	3	4.3308490E-03	2.1555508E-03	1.1222850E-03
3	1	4	8.1235580E-03	3.7430290E-03	1.8305379E-03
3	2	2	4.1978325E-03	2.0957366E-03	1.0940639E-03
3	2	3	7.5727270E-03	3.5116440E-03	1.7273180E-03
3	2	4	1.5504650E-02	6.5746310E-03	3.0051642E-03
3	3	3	1.4936222E-02	6.3525415E-03	2.9117440E-03
3	3	4	3.3597292E-02	1.2929522E-02	5.4516700E-03
3	4	4	8.3052490E-02	2.8703908E-02	1.1044052E-02

X = 40.0

K	M	N	A = 1.0	A = 1.2	A = 1.4
3	0	0	5.0429770E-03	2.7810115E-03	1.5780963E-03
3	0	1	7.7293880E-03	4.0276820E-03	2.1900222E-03
3	0	2	1.3349807E-02	6.4195315E-03	3.2879810E-03
3	0	3	2.6834659E-02	1.1574472E-02	5.4655530E-03
3	0	4	6.4455295E-02	2.4238564E-02	1.0308227E-02
3	1	1	1.2894110E-02	6.2269100E-03	3.2005540E-03
3	1	2	2.4768534E-02	1.0783257E-02	5.1326810E-03
3	1	3	5.6279640E-02	2.1462454E-02	9.2442835E-03
3	1	4	1.5351579E-01	5.0066115E-02	1.9092449E-02
3	2	2	5.3913990E-02	2.0649510E-02	8.9290590E-03
3	2	3	1.3997928E-01	4.6002205E-02	1.7673409E-02
3	2	4	4.3437408E-01	1.2042699E-01	4.0385605E-02
3	3	3	4.1475466E-01	1.1531224E-01	3.8786840E-02
3	3	4	1.4528997E+00	3.3826308E-01	9.8391465E-02
3	4	4	5.6727250E+00	1.1027709E+00	2.7605554E-01

X = 40.0

K	M	N	A = 1.6	A = 1.8	A = 2.0
3	0	0	9.1449915E-04	5.3855115E-04	3.2122525E-04
3	0	1	1.2274462E-03	7.0369105E-04	4.1055085E-04
3	0	2	1.7596820E-03	9.7250065E-04	5.5072290E-04
3	0	3	2.7474392E-03	1.4450252E-03	7.8623650E-04
3	0	4	4.7750680E-03	2.3533623E-03	1.2148496E-03
3	1	1	1.7179146E-03	9.5173970E-04	5.4008130E-04
3	1	2	2.5977180E-03	1.3741726E-03	7.5137045E-04
3	1	3	4.3309155E-03	2.1555594E-03	1.1222852E-03
3	1	4	8.1238560E-03	3.7430610E-03	1.8305405E-03
3	2	2	4.1978310E-03	2.0957416E-03	1.0940645E-03
3	2	3	7.5727190E-03	3.5116535E-03	1.7273192E-03
3	2	4	1.5504632E-02	6.5746635E-03	3.0051714E-03
3	3	3	1.4936202E-02	6.3525505E-03	2.9117447E-03
3	3	4	3.3597257E-02	1.2929537E-02	5.4516810E-03
3	4	4	8.3052565E-02	2.8703891E-02	1.1044121E-02

X = ∞

K	M	N	A = 1.0	A = 1.2	A = 1.4
3	0	0	5.0429770E-03	2.7810115E-03	1.5780963E-03
3	0	1	7.7293880E-03	4.0276820E-03	2.1900222E-03
3	0	2	1.3349807E-02	6.4195315E-03	3.2879810E-03
3	0	3	2.6834659E-02	1.1574472E-02	5.4655530E-03
3	0	4	6.4455295E-02	2.4238564E-02	1.0308227E-02
3	1	1	1.2894110E-02	6.2269100E-03	3.2005540E-03
3	1	2	2.4768534E-02	1.0783257E-02	5.1326810E-03
3	1	3	5.6279640E-02	2.1462454E-02	9.2442835E-03
3	1	4	1.5351579E-01	5.0066115E-02	1.9092449E-02
3	2	2	5.3913990E-02	2.0649510E-02	8.9290590E-03
3	2	3	1.3997928E-01	4.6002205E-02	1.7673409E-02
3	2	4	4.3437408E-01	1.2042699E-01	4.0385605E-02
3	3	3	4.1475466E-01	1.1531224E-01	3.8786840E-02
3	3	4	1.4528997E+00	3.3826308E-01	9.8391465E-02
3	4	4	5.6727250E+00	1.1027709E+00	2.7605554E-01

X = ∞

K	M	N	A = 1.6	A = 1.8	A = 2.0
3	0	0	9.1449915E-04	5.3855115E-04	3.2122525E-04
3	0	1	1.2274462E-03	7.0369105E-04	4.1055085E-04
3	0	2	1.7596820E-03	9.7250065E-04	5.5072290E-04
3	0	3	2.7474392E-03	1.4450252E-03	7.8623650E-04
3	0	4	4.7750680E-03	2.3533623E-03	1.2148496E-03
3	1	1	1.7179146E-03	9.5173970E-04	5.4008130E-04
3	1	2	2.5977180E-03	1.3741726E-03	7.5137045E-04
3	1	3	4.3309155E-03	2.1555594E-03	1.1222852E-03
3	1	4	8.1238560E-03	3.7430610E-03	1.8305405E-03
3	2	2	4.1978310E-03	2.0957416E-03	1.0940645E-03
3	2	3	7.5727190E-03	3.5116535E-03	1.7273192E-03
3	2	4	1.5504632E-02	6.5746635E-03	3.0051714E-03
3	3	3	1.4936202E-02	6.3525505E-03	2.9117447E-03
3	3	4	3.3597257E-02	1.2929537E-02	5.4516810E-03
3	4	4	8.3052565E-02	2.8703891E-02	1.1044121E-02

9.   BIBLIOGRAPHY

1. A. Michels, J. de Boer and A. Bijl, Physica, $\underline{4}$, 981, 1937.

2. W. Schottky, Phys. Z., $\underline{21}$, 232, 1920.

3. Nitrogen: R.J. Lunbeck, A. Michels and G.J. Wolkers,

            Appl. Sci. Res., $\underline{A3}$, 197, 1952;

    Hydrogen: A. Michels and M. Goudeket, Physica, $\underline{8}$, 347 & 387, 1941;

    Argon: A. Michels, R.J. Lunbeck and G.J. Wolkers,

            Appl. Sci. Res., $\underline{A2}$, 345, 1951;

    Helium: S.W. Akin, Trans. Am. Soc. Mech. Engrs., $\underline{72}$, 751, 1950.

4. A. Sommerfeld and H. Welker, Ann. Physik, $\underline{32}$, 56, 1938.

5. S.R. de Groot and C.A. ten Seldam, Physica, $\underline{12}$, 669, 1946.

6. T.L. Cottrell, Trans. Faraday Soc., $\underline{47}$, 337, 1951.

7. C.A. ten Seldam and S.R. de Groot, Physica, $\underline{18}$, 891 & 905, 1952.

8. T. Inui, Proc. Phys.-Math. Soc. Japan, $\underline{20}$, 770, 1938;

            ibid, $\underline{23}$, 992, 941.

9. A. Norsdieck, Phys. Rev., $\underline{58}$, 310, 1940.

10. M. Abramowitz and I.A. Stegun, Editors, Handbook of Mathematical

            Functions, AMS 55, National Bureau of Standards, 1965.

11. C. Zener and V. Guillemin, Phys. Rev., $\underline{34}$, 999, 1929.

12. J.H. Bartlett, Phys. Rev., $\underline{37}$, 507, 1931.

13. N. Rosen, Phys. Rev., $\underline{38}$, 255 & 2099, 1931.

14. M. Kotani, A. Amemiya, E. Ishiguro and T. Kimura,

            Table of Molecular Integrals, Maruzen Co. Ltd., Tokyo, 1955.

15. K. Rudenberg, J. Chem. Phys., $\underline{19}$, 1459, 1951.

16. A. Dalgarno, M.T.A.C., $\underline{8}$, 203, 1954.

17. J. Miller, J.M. Gerhauser and F.A. Matsen, Quantum Chemistry

            Integrals and Tables, University of Texas Press, 1958.

18. H.M. James and A.S. Coolidge, J. Chem. Phys., $\underline{1}$, 825, 1933.

19. J.H. Van Vleck, Theory of Electric and Magnetic Susceptibilities,
    Oxford University Press, New York, 1932.

20. W. Gordy, W.V. Smith and R. Trambarulo, Microwave Spectroscopy,
    Wiley, 1953.

21. A.D. May, V. Stryland, J.C. Degen and H.L. Welsh,
    Can. J. Phys., $\underline{39}$, 1769, 1961.

22. J.O. Hirschfelder, C.F. Curtiss and R.B. Bird, Molecular Theory of
    Gases and Liquids, Wiley, 1954.

23. H. Hellmann, Quantenchemie, Leipzig, Deutcke & Co., 1937.

24. R.P. Feynman, Phys. Rev., $\underline{36}$, 340, 1939.

25. T. Berlin, J. Chem. Phys., $\underline{19}$, 208, 1951.

26. T. Kihara, J. Phys. Soc. Japan, $\underline{6}$, 289, 1951.