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#### THEORETICAL THERMODYNAMIC PROPERTIES OF LOW TEMPERATURE FLUIDS

by

Zul Azhar Zahid Jamal

A Thesis Submitted to the Faculty of The Graduate College in partial fulfillment of the requirements for the Degree of Master of Arts Department of Physics

Western Michigan University Kalamazoo, Michigan December 1987

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#### THEORETICAL THERMODYNAMIC PROPERTIES OF LOW TEMPERATURE FLUIDS

Zul Azhar Zahid Jamal, M.A. Western Michigan University, 1987

The thermodynamic functions for low temperature fluids are computed using parametric integral equations and perturbation theory. Parametric integral equation N is applied to a low temperature Lennard-Jones gas. It is found that there is no significant improvement over the better known parametric integral equation C. The two parameter integral equation T is applied to a low temperature square-well potential and is found to be unsatisfactory at reduced temperatures of T\* = 1.4 and 1.6, but guite accurate at  $T^* = 2.2$ . The equation T results for T\* = 2.2 are used as the reference system in perturbation theory computations. Tables of (reduced) pressure, internal energy, entropy, enthalpy, Helmholtz energy, and Gibbs energy are constructed for reduced density n\* < 0.85, and reduced temperature 0.7 < T\* < 2.15. The results of reduced pressure agree very well with the molecular dynamic results but results of reduced internal energy deviate from the accepted values for large perturbations.

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Zul Azhar Zahid Jamal

Order Number 1332222

# Theoretical thermodynamic properties of low temperature fluids

Zahid Jamal, Zul Azhar Bin, M.A.

Western Michigan University, 1987



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#### CHAPTER I

#### INTRODUCTION

A fundamental problem in statistical mechanics is to compute the thermodynamic properties of a material. In this research integral equation methods and perturbation theory are used to compute the thermodynamic functions of simple classical fluids at low temperatures. Results which are presented include the values of pressure, internal energy, entropy, enthalpy, Helmholtz energy, and Gibbs energy.

#### The System

In a simple classical fluid, it is assumed that the system consists of particles which interact with pairwise radial forces. These forces depend only on the separation distance of the pair of particles for which classical mechanics is good enough to describe the system. The Hamiltonian of a simple classical fluid is given by

$$H = K + \frac{1}{2} = K + \frac{1}{2} \sum_{i=1}^{2} \frac{0}{i} (rij), \qquad (1)$$

where K is the kinetic energy of the particles and  $\oint$  is the potential energy of the particles which includes the sum of the pair energy of particles  $\emptyset$ (rij) where rij is the distance between particles i and j.

The Lennard-Jones pair potential studied here is of the form<sup>1</sup>

$$\emptyset(r) = 4 \in [(\sigma/r)^{12} - (\sigma/r)^{6}], \qquad (2)$$

where  $\boldsymbol{\epsilon}$  and  $\boldsymbol{\sigma}$  are parameters characteristic of the molecules which make up the system.

The square-well potential studied here is of the  $\ensuremath{\mathsf{form}^2}$ 

$$\emptyset(\mathbf{r}) = \infty, \mathbf{r} < \mathbf{d},$$
 $\emptyset(\mathbf{r}) = -\mathbf{e}, \mathbf{d} \le \mathbf{r} \le 1.5 \, \mathbf{d},$ 
 $\emptyset(\mathbf{r}) = 0, \mathbf{r} > 1.5 \, \mathbf{d},$ 
(3)

where  $\boldsymbol{\epsilon}$  is the well depth and d is the diameter of the hard-sphere core.

# Radial Distribution Function

The radial distribution function is defined by

$$g(\mathbf{r}) = \underline{\mathbf{n}(\mathbf{r})}_{\overline{\mathbf{n}}}, \qquad (4)$$

where n(r) is the average number of particles per unit volume at a distance r from a central particle and  $\vec{n}$  is the average number density which is the total number of particles divided by the volume of the system ( $\vec{n} = N/V$ ). In terms of potential energy, g(r) can be written as<sup>3</sup>

:

$$g(r) = V^2 Z^{-1} \int \dots \int exp (-\phi/kT) dr_3 \dots dr_N$$
, (5)  
 $Z = \int \dots \int exp (-\phi/kT) dr_1 \dots dr_N$ ,

where k is the Boltzmann's constant and T is the absolute temperature. The integration is over the position coordinates of the particles. Figure 1 shows a typical shape of a radial distribution function.



Figure 1. Graph of Radial Distribution Function as a Function of Particle Separation x for  $n^* = 0.80$ at  $T^* = 1.6$  (For Parametric Integral Equation T with Parameters  $b_2 = -1.80$  and  $b_3 = 0.55$ )

Once g(r) is known, the pressure (P) and internal energy (U) can be computed by the following relation-

ships<sup>4</sup>

$$P^{\star} = \frac{PV}{NkT} = 1 - \frac{2\pi N}{3VkT} \int_{0}^{\infty} \frac{d\theta}{dr} gr^{3} dr , \qquad (6)$$

and

$$U^{\star} = \frac{2U}{3NkT} = 1 + \frac{4\pi N}{3VkT} \int_{0}^{\infty} gr^{2} dr . \qquad (7)$$

When the pressure and internal energy are computed over a range of temperatures and densities, it is possible to compute other thermodynamic functions. Therefore, g(r) contains a complete thermodynamic description of the system.

#### CHAPTER II

#### METHODS FOR COMPUTING THERMODYNAMIC FUNCTIONS

#### Exact Methods

The most direct way of computing g(r) (thus getting the thermodynamic functions) is by a method called molecular dynamics<sup>5</sup> (MD). Here Newton's equations of motion are solved on a computer to obtain the motions of the particles. Then relevant averages that are related to the thermodynamic properties are computed. Another method is called Monte Carlo<sup>6</sup> (MC). In this method the motions of the particles are governed by probability rules and averages related to the thermodynamic properties can be computed. Both methods are very direct, therefore these results are often called "exact" (however there are approximations involved) and are used as the accepted values. The main disadvantage of these methods are large computer and long computer time requirements. In this research, the molecular dynamics results of Alder, Young, and Mark<sup>7</sup> are used for comparison for the square-well system.

#### Integral Equations

Integral equations are approximate equations for computing radial distribution function. Most give good results at low densities and high temperatures but produce large errors at high densities and low temperatures. The advantage of integral equations is the shorter computer time requirements compared to the "exact" methods.

Integral equations of interest here are the hypernetted chain<sup>8</sup> (HNC), Percus-Yevick<sup>9</sup> (PY), and parametric integral equations. Three parametric integral equations that have been studied are equation  $C_{10}$  equation N,<sup>11</sup> and equation T.<sup>12</sup> These integral equations are given by the Ornstein-Zernike equation,<sup>13</sup>

h(12) = c(12) + 
$$\bar{n} \int c(13)h(23)d3$$
, (8)  
where

$$h = g - 1.$$
 (9)

The function h is the total correlation function and the function c is the direct correlation function. (12) indicates the correlation of particle 1 on particle 2 and the same apply to (13) and (23). In terms of the direct correlation function, the integral equations are given by

(HNC) 
$$c = g - 1 - \ln (ge^{\beta \phi})$$
, (10)

(PY) 
$$c = g (1 - e^{\phi \phi})$$
, (11)

(Equation C)  $c = g - 1 - \frac{1}{a} \ln (age^{\frac{59}{2}} - a + 1)$ , (12)

(Equation N) 
$$c = g - 1 - \frac{1 - ge^{\frac{2}{9}\phi}}{ge^{\frac{2}{9}\phi}(a-1) - a}$$
, (13)

where  $\beta = (kT)^{-1}$  and a is an adjustable parameter. There is no simple relationship between c and g for equation T.

& function S is introduced,

$$S = h - c. \tag{14}$$

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Using this and equation (8), the integral equations can be written as

$$(PY) \quad g = e^{-\beta \phi} \quad (1 + S), \qquad (15)$$

$$(HNC) \quad g = e^{-\beta \phi} e^{S}$$

$$= e^{-\beta \phi} [1 + S + (1/2)S^{2} + (1/6)S^{3} + ...], \quad (16)$$

$$(Equation C) \quad g = e^{-\beta \phi} [1 + 1/a \ (e^{aS} - 1)]$$

$$= e^{-\beta \phi} [1 + S + (1/2)aS^{2} + (1/6)a^{2}S^{3} + ...), \quad (17)$$

$$(Equation N) \quad g = \frac{e^{-\beta \phi} (1 + aS)}{1 + aS - S}$$

$$= e^{-\beta \phi} [1 + S + (1 - a)S^{2} + (1 - a)^{2}S^{3} + ...], \quad (18)$$

$$(Equation T) \quad g = e^{-\beta \phi} (1 + S + b_{2}S^{2} + b_{3}S^{3}). \quad (19)$$

where  $a_1$ ,  $b_2$ , and  $b_3$  are adjustable parameters.

In this research parametric equation N is studied for a low temperature Lennard-Jones gas and equation T is solved for g for three temperatures and for several densities and sets of parameters.

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The first order perturbation theory of Zwanzig<sup>14</sup> will be considered. Here the pair potential energy is separated into sum of a reference potential  $\theta_r$  and perturbing potential  $\theta_p$ ,

$$\emptyset = \emptyset_r + \emptyset_p. \tag{20}$$

The system Helmholtz free energy (F) and the reference Helmholtz free energy (F<sub>r</sub>) are related by<sup>15</sup>

$$F = F_r + F_p = F_r + \frac{N^2}{2V} \int_0^\infty g_r 4\pi r^2 dr.$$
 (21)

The thermodynamic functions can then be calculated from the  $g_r$  and the correction terms involving the perturbation potential. Results of equation T are used in this research to calculate the thermodynamic functions of the reference system.

#### CHAPTER III

#### COMPUTATIONAL METHOD

#### Solutions of Equation N

The method of solution of equation N is essentially that of Broyles.<sup>16</sup> This involves an iterative procedure where equation N is solved numerically on a computer to obtain the radial distribution function.

The following dimensionless quantities are introduced for the Lennard-Jones pair potential,

$$\mathbf{x} = \mathbf{r}/\mathbf{\sigma} , \qquad (22)$$

$$T^* = kT/\epsilon = 1/\beta\epsilon$$
, (23)

$$\mathbf{n}^{\star} = \mathbf{\hat{n}} \mathbf{d}^3 \quad (24)$$

Equations (6) and (7) can then be written  $as^{17}$ 

$$P^{\star} = 1 - \frac{16\pi n^{\star}}{T^{\star}} \int_{0}^{\infty} (x^{-10} - 2 x^{-10}) g(x) dx , \qquad (25)$$

and

$$U^{*} = 1 + \frac{16\pi n^{*}}{3T^{*}} \int_{0}^{\infty} (x^{-10} - x^{-4}) g(x) dx . \qquad (26)$$

The computer gives solutions for 75 points with an x interval of 0.075 and for 297 points with an x interval of 0.01875. Solutions of 297 points will only be considered. The truncation point is at x = 5.55.

The computational steps are as follows,

- 1) Equation N is solved for the isotherm T\* = 1.6 at reduced densities of n\* = 0.70 and n\* = 0.90. Several different values of the parameter a are used.
- 2) Graphs of P\* versus a for both the reduced densities are then drawn. Here, results by D. D. Carley<sup>18</sup> using integral equations combined with perturbation theory are used for comparison.

#### Solutions of Equation T

The method of solution here is the same as the method of solving equation N. The same dimensionless quantities are introduced except for the square-well,

$$x = r/d$$
, (27)

$$n^* = Nd^3/V$$
 (28)

0 0

P\* and U\* can then be written  $as^{19}$ 

$$P^* = 1 + (2/3)\pi n^* [g(1.0) - 3.375 g(1.5) (1-e^{3e})], (29)$$

$$U^{*} = 1 - \frac{4\pi n^{*}}{3T^{*}} \int_{1.0}^{1.5} g(x) x^{2} dx , \qquad (30)$$

where g(1.0) is the radial distribution function as x approaches 1.0 from above and g(1.5) is the radial distribution function as x approaches 1.5 from below.

The computer gives solutions for 75 points with an x interval of 0.07142857 and for 297 points with an x

interval of 0.01785714. As before, solutions of 297 points will only be considered. The truncation point is at x = 5.2857.

The computational steps of equation T are as follows:

- Equation T is solved for the isotherms T\* = 1.4,
   1.6, and 2.2 at a high and an intermediate density.
   Different sets of parameters are used so that a grid can be set up for the parameters (b<sub>2</sub> and b<sub>3</sub>).
- 2) With the above results, a least square-fit computer program is used to determine the c's that give the best least square fit according to the equation  $P^* = P_0 + c_1b_2 + c_2b_3 + c_3b_2^2 + c_4b_3^2 + c_5b_2b_3$ . (31)
- 3) A computer program is then used to find values of b<sub>2</sub> and b<sub>3</sub> that give results equal to the accepted results. Molecular dynamics results of Alder are used for comparison. A graph of b<sub>3</sub> versus b<sub>2</sub> is then plotted, and the point of interception is taken to be the best choice of parameters for the isotherm. Since equation (31) is approximate, equation T is solved with these "best" values to see if indeed they give agreement with accepted values of P\*.
- 4) Equation T is solved again at other densities, using the best choice of parameters. With the results, another computer program is then used to obtain the

interpotation coefficients (Pade coefficients) which can then be used to find the values for other densities without going through the long iteration procedure again. The two interpolation formulas for P\* and U\* are

$$p^{*} = 1 + a_{1}n^{*} + a_{2}n^{*2} + a_{3}n^{*3}$$
(32)  
$$1 + a_{4}n^{*} + a_{5}n^{*2} + a_{6}n^{*3},$$

and

$$U^* = 1 + a_1 n^* + a_2 n^{*2} + a_3 n^{*3}$$
(33)  
$$\frac{1 + a_4 n^* + a_5 n^{*2} + a_6 n^{*3}}{1 + a_4 n^* + a_5 n^{*2} + a_6 n^{*3}}.$$

The results for pressure only are used in determining the best choice of parameters because results in the internal energy are not as sensitive to changes in the parameters.

#### Computation of Thermodynamic Functions (Perturbation Method)

The reference potential is taken to be

$\theta_{r}(r) = \infty$	, r < d ,	(34)
$\emptyset_r(r) = -\infty \epsilon$	, $d \leq r \leq 1.5 d$ ,	
$\theta_{r}(r) = 0$	, r > 1.5 d ,	

where  $\propto$  is a constant.

The following dimensionless quantities are introduced,

$$\mathbf{T}^+ = \mathbf{T}^* / \boldsymbol{\alpha} , \qquad (35)$$

 $F^* = 2F/3NkT.$  (36)

The system and the reference system are then both square-well where in the well

$$\emptyset/kT = -1/T*$$
, (37)

$$\theta_{\rm r}/kT = -1/T^{+} \,. \tag{38}$$

P\* and U\* are related by the following equation<sup>20</sup>

$$dF^{\star} = \left(\frac{2P^{\star}}{3n^{\star}}\right) dn^{\star} - \left(\frac{U^{\star}}{T^{\star}}\right) dT^{\star} .$$
(39)

Equation 21 can be written as

$$F^{*} = F_{r}^{*} + F_{p}^{*} = F_{r}^{*} + \frac{4\pi n^{*} (\alpha - 1)}{3T^{*}} \int_{1.0}^{1.5} g_{r}(x) x^{2} dx. \quad (40)$$

Comparison of the above equation with equation 30 will show that

$$F_{p}^{\star} = \left(1 - \frac{T^{\dagger}}{T^{\star}}\right) \left(1 - U_{r}^{\star}\right) .$$
(41)

Equations 39, 40, and 41 are the basic equations that are used to compute the thermodynamic functions.

A computer program by D. D. Carley and modified by Z. Z. Jamal is used to do the computations. The program does computations at reference temperature  $T^* = 2.2$  and the thermodynamic functions are constructed for  $0.7 \leq T^*$  $\leq 2.15$ , and  $0.05 \leq n^* \leq 0.85$  for an interval of 0.05. The computational steps in the program are as follows: 1)  $T^* = 20.0$ ,  $n^* = 0.001$  is taken to be the standard

state and F\* in that state is denoted by 
$$F_0^*$$
.

Equation 39 is then integrated at  $n^* = 0.001$ , using the approximation  $g = e^{-\beta \phi}$  at this low density. The result will be 21

$$F^* - F_0^* = - \int_{20.0}^{T^*} \left(1 - \frac{9.5 \times 10^{-3} \pi}{9T^*}\right) \frac{dT^*}{T^*}.$$
 (42)

In the proceeding steps  $F^* - F_0^*$  will be denoted as  $F^*$  (n\* = 0.001, T\*).

2)  $F_r^*$  (n\* = 0.001, T\*) can now be computed using equations 40 and 41, resulting in

$$F_{r}^{*}(n^{*}=0.001, T^{*}) = F^{*}(n^{*}=0.001, T^{*}) - \left(1 - \frac{T^{+}}{T^{*}}\right) \left(1 - U_{r}^{*}\right)$$
(43)

3) Equation 39 is integrated again at a constant T\*.  $F_{r}$ \* (n\*,T\*) can then be computed by the following equation,

$$F_{r}^{*}(n^{*},T^{*}) = F_{r}^{*}(n^{*} = 0.001,T^{*}) + \begin{pmatrix} n^{*} \\ .001 \end{pmatrix} \begin{pmatrix} 2P^{*} \\ 3n^{*} \end{pmatrix} dn^{*}.$$
 (44)

For low densities (n\*  $\leq$  0.10), the values of P\* are interpolated values in the form

$$P^* = 1 + b_1 n^* + b_2 n^{*2} + b_3 n^{*3} .$$
 (45)

The integral can then be done analytically. At higher densities, interpolated values of P\* are in the form of equation 32. Here numerical integration must be used.

4)  $F_{p}^{*}$  (n\*,T\*) can be computed directly from equation 41. 5) Finally, with  $F_r^*$  and  $F_p^*$  known,  $F^*$  (n\*, T\*) is obtained from the relationship

$$F^* = F_r^* + F_p^*$$
 (46)

6) Numerical differentiation is then used to compute P\* and U\* as

$$P^{\star} = \frac{3}{2} n^{\star} \left( \frac{\partial F^{\star}}{\partial n^{\star}} \right) , \qquad (47)$$

and

$$U = -T^{*}\left(\frac{\partial F^{*}}{\partial T^{*}}\right)$$
 (48)

7) Other thermodynamic functions can easily be obtained by the following thermodynamic relationships<sup>22</sup>

$$S^* = 2 S/3Nk = U^* - F^*,$$
 (49)

$$H^* = 2 H/3NkT = U^* + (2/3) P^*$$
, (50)

and

$$G^* = 2 G/3NkT = F^* + (2/3) P^*$$
, (51)

where S is the entropy, H is the enthalpy, and G is the Gibbs energy.

#### CHAPTER IV

#### **RESULTS AND COMPARISONS**

#### Parametric Integral Equation N and The Lennard-Jones Potential

For the Lennard-Jones potential, equation N was solved for the isotherm  $T^* = 1.6$  at reduced densities of  $n^* = 0.70$  and  $n^* = 0.90$  for several different values of the parameter a. Results of P\* and U\* obtained can be found in the appendix. Graphs of P\* versus a were then drawn. The accepted values for the isotherm  $T^* = 1.6$  are  $P^* = 1.77$  at  $n^* = 0.70$ , and  $P^* = 4.61$  at  $n^* = 0.90$ (Results by Carley using integral equations combined with perturbation theory). The accepted values were also shown on the graphs (see figure 2).

It can be seen clearly that there is no single parameter a that give P\* values equal to the accepted P\* values at both the reduced densities. Thus equation N does not produce good results.



#### Parametric Integral Equation T and the Square-Well Potential

For the square-well, equation T was solved at T\* = 1.4, 1.6, and 2.2 which were above the critical temperature. These choices of T\* were to keep the perturbation as small as possible while still providing good thermodynamic values for the reference system (for the perturbation theory computations).

The first thing that was done was to solve equation T for  $T^* = 1.4$  at  $n^* = 0.70$ , and  $n^* = 0.88$  with different sets of the parameters  $b_2$  and  $b_3$ . At  $n^* = 0.88$  the results of P\* obtained were unsatisfactory. Computations were done again at  $n^* = 0.85$  and the results of P\* obtained were still unsatisfactory. The same problem occurred when equation T was solved at  $T^* = 1.6$ . Therefore at  $T^* = 1.4$  and 1.6, equation T was found to be unsatisfactory. The results of P\* and U\* can be found in the appendix.

Equation T was then solved for the isotherm  $T^* = 2.2$ at  $n^* = 0.65$ , and  $n^* = 0.85$  with different sets of the parameters  $b_2$  and  $b_3$ . The P\* and U\* results obtained were satisfactory and can be found in the appendix. The results were then used with a least squares program to find the coefficients in equation 31. Table 1 gives the values of these coefficients.

C	oefficients	for Least	Square Equ	ation at T*	= 2.2
n*	cl	c2	c3	C4	¢5
0.65	.819257	.825071	573483	39785	-1.14248
0.85	5.70092	11.345	.193985	-23.4007	-14.7053

Table 1

The coefficients were used to compute various values of  $b_2$  and  $b_3$  that give P\* results equal to the accepted P\* results which were taken from the extrapolated and interpolated results of Alder. Graphs of  $b_3$ versus  $b_2$  were then drawn for both the reduced densities. The point of interception ( $b_2 = -0.517$ ,  $b_3 =$ 0.208) gives the best choice of parameters (see figure 3).

The best choice of parameters was then used to solve equation T again at ten other densities along the isotherm. The results are given in Table 3. Here, values of P\* and U\* are rounded off and only the 297 points are taken. A more complete result can be found in the appendix.

Results in Table 3 were applied to the interpolation formulas for P\* and U\* (equations 32 and 33) to obtain the Pade coefficients. Other interpolated results of P\* and U\* were then easily obtained without going through the long procedure again. The Pade coefficients are given in Table 4 and the other interpolated results of P\*



Figure 3. Parameters  $b_3$  and  $b_2$  at  $T^* = 2.2$  The Numbers Near the Curves are the Densities  $(n^*)$ 

and U\* are given in Table 5.

The results in Table 5 were used to plot graphs of P\* versus n\*, and U\* versus n\*. Interpolated and extrapolated results of Alder were also plotted on the graphs for comparison (see figure 4 and figure 5). The agreement is quite good, thus equation T produces good results.

Та	b	1	е	2
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n*	P*	Ű*
.001	0.9992342	0.9976260
.01	0.992544	0.976332
.10	0.94806	0.77045
.20	0.9576	0.5539
.30	1.05	0.342
.50	1.67	-0.0959
.60	2.31	-0.322
.65	2.77	-0.434
.80	5.23	-0.734
.85	6.74	-0.811

Equation T Results at T\* = 2.2 (b<sub>2</sub> = 0.208, b<sub>3</sub> = -0.517)

Т	ab	le	3
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Pade Coefficients for  $P^*$  and  $U^*$  for  $T^* = 2.2$ 

Coefficients	p*	U*	
 al	-3.38456	-3.97487	
a2	5.94679	5.45626	
ag	-5.10293	-3.37914	
ag	-2.61652	-1.59996	
a5	1.69642	.733093	
aß	175072	.750641	

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n*	P*	U*	
•05	.967498	.883214	
.10	.94806	.7702	
.15	.94395	.6606	
.20	.958	.554	
.25	.993	.449	
.30	1.05	.345	
• 35	1.14	.239	
.40	1.27	.131	
.45	1.44	.0188	
.50	1.66	0964	
.55	1.94	212	
.60	2.30	326	
.65	2.77	434	
.70	3.38	537	
.75	4.17	634	
. 80	5.25	725	
.85	6.75	812	

Table 4

Interpotated Results at T\* = 2.2



Figure 4. P\* versus n\* at T\* = 2.2 The Points are the Accepted Results of Alder



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# Perturbation Theory Applied to the Square-Well Potential

A computer program was used to compute the thermodynamic functions. The program was modified to do computations at a reference temperature of  $T^* = 2.2$ . Results of the reduced internal energy (Table 5) and the Pade coefficients for the pressure (Table 4) were used in the program for the reference part computations.

The thermodynamic functions obtained were for 0.7  $\leq$ T\*  $\leq$  2.15 and 0.05  $\leq$  n\*  $\leq$  0.85 for an interval of 0.05. The results of T\* = 0.85, 1.05, 1.35, 1.55, and 2.10 will only be discussed here. A complete result of the thermodynamic functions can be found in the appendix.

Graphs of P\* versus n\* and U\* versus n\* were plotted for the selected T\*. As before, interpolated and extrapolated results of Alder were shown in the graphs for comparisons. Results at n\* = 0.05 were dropped from the graphs because of numerical error  $^{23}$  in the numerical differentiation computations of P\* and U\*. These graphs are shown in figures 6-9. In addition, graphs of F\*, S\*, H\*, and G\* versus n\* were also plotted (figures 10-13).

From these graphs, it can be seen that the P\* results agree quite well with the accepted results. However, the U\* results do not agree with the accepted results at lower temperatures but agree very well at higher temperatures.

For further comparisons, graphs of P\* and U\* versus  $n^* = 0.85$ , 0.65, and 0.45 were plotted together with the interpolated and extrapolated results of Alder (figures 14-19).

Again, it can be seen that good agreements with the accepted results are only at higher temperatures.



Figure 6. P\* versus n\* for T\* = 0.85, 1.05, and 1.35. The Numbers Near the Curves are the Temperatures (T\*) and the Points are the Accepted Results of Alder.


Figure 7. P\* versus n\* for T\* = 1.55 and 2.10. The Numbers Near the Curves are the Temperatures (T\*) and the Points are the Accepted Results of Alder.



Figure 8. U\* versus n\* for T\* = 0.85, 1.05, and 1.35. The Numbers Near the Curves are the Temperatures (T\*) and the Points are the Accepted Results of Alder.



Figure 9. U\* versus n\* for T\* = 1.55 and 2.10. The Numbers Near the Curves are the Temperatures (T\*) and the Points are the Accepted Results of Alder



Figure 10. F\* versus n\* for Constant T\*. The Numbers Near the Curves are the Temperatures (T\*)





Figure 12. H\* versus n\* for Constant T\*. The Numbers Near the Curves are the Temperatures (T\*)



Figure 13. G\* versus n\* for Constant T\*. The Numbers Near the Curves are the Temperatures (T\*)



Figure 14. P\* versus T\* for n\* = 0.85. The Points are the Accepted Results of Alder



Figure 15. P\* versus T\* for n\* = 0.65. The Points are the Accepted Results of Alder



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Figure 16. P\* versus T\* for n\* = 0.45. The Points are the Accepted Results of Alder



Figure 17. U\* versus T\* for n\* = 0.85. The Points are the Accepted Results of Alder



Figure 18. U\* versus T\* for n\* = 0.65. The Points are the Accepted Results of Alder



Figure 19. U\* versus T\* for n\* = 0.45. The Points are the Accepted Results of Alder

#### CHAPTER V

#### SUMMARY AND CONCLUSIONS

In the first part of this research, equation N, a one parameter integral equation, was solved for a Lennard-Jones potential at T\* = 1.6. It was found out that there was no single parameter that produced P\* results equal to the accepted P\* results at a high and intermediate density. Thus equation N results have no better improvement over equation C.

In the second part of this research, equation T was solved for a square-well potential at  $T^* = 1.4$ , 1.6, and 2.2. The choices of  $T^*$  were to keep the perturbation as small as possible but still provide good thermodynamic values. At  $T^* = 1.4$  and 1.6, the best choice of parameters were difficult to determine and thus the P\* results obtained were unsatisfactory. However at  $T^* =$ 2.2, the P\* and U\* results obtained were in good agreement with the accepted results.

The last part of this research was to compute the thermodynamic functions of a square-well potential using the first order perturbation theory. Equation T results at  $T^* = 2.2$  were used as the reference system. In summary, the agreement with the accepted results was

found to be fairly good for P\* results in all the densities tried (n\* = 0.45, 0.65, and 0.85) and for U\* the results deviate from the accepted results for large perturbations.

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APPENDICES

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#### APPENDIX A

### SOLUTIONS OF EQUATION N FOR THE LENNARD-JONES POTENTIAL

The following notations are used:

а	Value of the parameter.
n*	Value of the reduced density.
Τ*	Value of the reduced temperature.
N	An A in the column indicates the
	computer gives solutions for 75 points
	with an x interval of 0.075. A B
	indicates solutions for 297 points
	with an x interval of 0.01875.
SDSS	A measurement of the difference
	between the final guessed value for S
	and computed value of S. A smaller
	value of SDSS shows a better conver-
	gence.
P*	Value of the reduced pressure.

U\* Value of the reduced internal energy.

TA	B	L	Е	- 5
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No.	a	T*	n*	N	SDSS	p*	Ü*
1	1.0	1.60	0.70	A	.53E-7	1.9324967	-0.875351433
2				В	.19E-6	1.9980859	-0.87126613
3	1.05			A	.25E-7	1.8937119	-0.87965620
4				в	.13E-6	1.9564418	-0.87592185
5	1.10			A	.71E-7	1.8564243	-0.88377237
6				в	.97E-7	1,9165158	-0.88036036
7	1.20			A	.25E-7	1.7860041	-0.89148998
8				B	.17E-6	1.8413405	-0.88865137
9	1.30			A	.27E-7	1.7205099	-0.89859486
10				в	.20E-6	1.7716719	-0.89625132
11	1.40			A	.15E-6	1.6593699	-0.90516150
12				в	.15E-6	1,7068421	-0.90324891
13	1.50			A	.49E-7	1.6020926	-0.91124988
14				В	.16E-6	1.6462976	-0.90971720
15	1.0	1.60	0.90	A	.28E-6	4.7016106	-1.2821085
16				в	.44E-6	4.8757114	-1.2677398
17	1.10			A	.30E-6	4.4014683	-1.3177240
18				в	.48E-6	4.5532546	-1.3063517
19	1.20			A	.13E-6	4.1328001	-1.3491311
20				в	.50E-6	4.2670045	-1.3401062
21	1.30			A	.37E-6	3.8897307	-1.3771310
22				в	.37E-6	4.0096164	-1.3699915

Solutions of Equation N for a Lennard-Jones Potential at T\* = 1.6

No.	a	Т*	n*	N	SDSS	P*	U*
23	1.40			A	.43E-6	3.6681569	-1.4022915
24				в	.49E-6	3.7760890	-1.3967102
25	1.50			A	.31E-6	3.4649289	-1.4250360
26				в	.35E-6	3.5626028	-1.4207706
27	1.35			в	<b>.</b> 52E-6	3.8900108	-1.3837137

#### APPENDIX B

### SOLUTIONS OF EQUATION T FOR THE SQUARE-WELL POTENTIAL

The following notations are used:

b2, b3	Values of the parameters.
n*	Value of the reduced density.
Ţ <b>★</b>	Value of the reduced temperature.
N	An A in the column indicates the computer
	gives solutions for 75 points with an x
	interval of 0.07142857. A B indicates
	solutions for 297 points with an x
	interval of 0.01785714.
enee	A measurement of the difference between

- SDSS A measurement of the difference between the final guessed value for S and computed value of S. A smaller value of SDSS shows a better convergence.
- P\* Value of the reduced pressure.
- U\* Value of the reduced internal energy.

Т	A	B	L	E	6
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No.	Ъ2	b3	n*	N	SDSS	p*	U*
1	0	0	0.70	A	.17E-6	2.7064407	-1.4663641
2				в	.19E-6	2.9033673	-1.4576738
3	0	0.25		A	.lle-6	2.8045580	-1.4600754
4				в	.28E-6	3.0355175	-1.4509859
5	0	-0.25		A	.13E-6	2.5920277	-1.4739590
6				в	.34E-6	2.7505019	-1.4658368
7	-0.5	0.25		A	.22E-6	2.5974386	-1.4473672
8				В	.39E-6	2.7413003	-1.4379199
9	-0.5	0		A	.17E-6	2.4717321	-1.4518716
10				В	.41E-6	2.5727146	-1.4425888
11	-0.5	-0.25		A	.22E-6	2.3192363	-1.4570236
12				В	.34E-6	2.3715045	-1.4479239
13	-0.5	-0.5		A	.15E-6	2.1222067	-1.4631271
14				В	.36E-6	2.1185274	-1.4542048
15	0	0	0.88	A	.42E-6	6.1765938	-1.9693773
16				в	.52E-6	6.7654791	-1.9444580
17	0.5	0.25		A	.81E-5	7.5623784	-2.0038664
18	0.5	0		A	.28E-6	7.4417601	-2.0691860
19	0	0	0.85	A	.36E-6	5.4541945	-1.8960519
20	0	0	0.88	A	.39E-6	6.1765985	-1.9693773
21				B	.53E-6	6.7654681	-1.9444544
22	0	0.25		A	.21E-6	6.7746091	-1.9537644

Solutions of Equation T for a Square-Well Potential at  $T^* = 1.4$ 

No.	b <sub>2</sub>	b3	n*	N	SDSS	P*	U*
23				в	.50E-6	7.7979069	-1.9274399
24	0	-0.2		A	.50E-6	4.9812193	-1.9886978
25				в	•57E-6	4.8585720	-1.9659817
26	-0.2	0		A	.26E-6	5.5312147	-1.9549901
27				B	.50E-6	5.8377342	-1.9289298
28	-0.2	0.25		A	.25E-6	6.4254527	-1.9420483
29	0.2	-0.2		A	.37E-6	6.0312080	-2.0223064
30				в	.68E-6	6.3811374	-2.0052435
31	0.2	0		A	.46E-6	6.6619229	-1.9907377
32				в	.12E-5	7.4946079	-1.9676728
33	-0.5	-0.6	0.70	A	.17E-6	2.0223114	-1.4659705
34				в	.26E-6	1.9942538	-1.4570966
35	-0.7	-0.5		A	.17E-6	1.8423142	-1.4608274
36				в	.25E-6	1.7787014	-1.4514461
37	-0.3	-0.7		A	.13E-6	2.1327565	-1.4751508
38				в	.27E-6	2.1341805	-1.4670484
39	-0.3	-0.6		A	.17E-6	2.2184818	-1.4717984
40				в	.28E-6	2.2432756	-1.4635062
41	-0.6	-0.4		A	.14E-6	2.1062858	-1.4587924
42				в	.32E-6	2.0989339	-1.449648
43	-0.1	0.1	0.88	A	.25E-6	6.2390976	-1.9553459
44				в	.45E-6	6.9311752	-1.9292428
45	-1.22	0.395	0.70	A	.14E-6	2.1167855	-1.4396601
46				в	.18E-6	2.1376228	-1.4302590

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No.	b2	b3	n*	N	SDSS	P*	U*
47	-1.22	0.395	0.88	A	.42E-6	5.8535619	-1.9307692
48				в	.66E-6	8.8528786	-1.8994110
49				в	.66E-6	8.8528652	-1.8994167
50	-1.07	.175	0.70	в	.22E-6	2.0935967	-1.4342330
51	-1.15	0.30	0.88	в	.84E-6	11.539763	-1.9391854
52	-1.28	0.475		в	.48E-6	8.3722029	-1.8859012
53	-1.30	0.55		B	.59E-6	7.9984784	-1.8763876
54	-1.36	0.590		в	.62E-6	8.3181372	-1.8742921
55	-1.50	0.790		в	.49E-6	8.7128019	-1.8617127
56	-1.18	0.317		в	.75E-6	11.494004	-1.9351859
57	-0.4	0.2		A	.35E-6	5.8305979	-1.9349115
58				в	.45E-6	6.4600992	-1.9071889
59	-0.8	0.2		A	.34E-6	4.2083640	-1.9315255
60				в	.84E-6	5.0330834	-1.9030116
61	-0.8	0.4		A	.23E-6	5.6594925	-1.9151607
62				в	.57E-6	6.5751591	-1.8854182
63	-1.0	0.4		A	.36E-6	5.2838235	-1.9139934
64				в	.62E-6	6.4841747	-1.8834713
65	-1.0	0.6	0.88	A	.28E-6	6.0081081	-1.9043348
66				в	.54E-6	7.3034940	-1.8735385
67	-2.045	1.58		в	.51E-6	10.469301	-1.8324115
68	-1.2	0.7		В	.53E-6	7.7033939	-1.8667598
69	-1.5	0.6		В	.68E-6	9.8892717	-1.8807869
70	0	0	0.85	A	.31E-6	5.4541864	-1.8960524

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No.	b2	b3	n*	N	SDSS	P*	U*
71				в	.29E-6	5.9487872	-1.8753588
72	0	0.25		A	.18E-6	5.9152632	-1.8815556
73				в	.36E-6	6.7116704	-1.8596077
74	0	-0.25		A	.46E-6	4.4262424	-1.9187689
75				в	.41E-6	4.3592019	-1.9003787
76	-0.5	0.25		A	.18E-6	5.0541596	-1.8612123
<b>7</b> 7				B	.48E-6	5.5420351	-1.8379946
78	-0.5	0.4		A	.18E-6	5.4383440	-1.8553612
79				В	.42E-6	6.1353631	-1.8317640
80	-0.8	0.3		A	.33E-6	4.4449639	-1.8555832
81				В	.52E-6	4.8830867	-1.8318958
82	-0.8	0.6		A	.24E-6	5.4092269	-1.8423016
83				B	.48E-6	6.2571235	-1.8176932
84	-1.0	0.7		A	.25E-6	5.3592734	-1.8363988
85				В	.38E-6	6.3261275	-1.8112268
86	-1.0	0.5		A	.36E~6	4.8328004	-1.8446145
87				B	.43E-6	5.6197248	-1.8199499
88	-1.2	0.6		A	.26E-6	4.8810878	-1.8408585
89				в	.48E-6	5.9675555	-1.8156517
<b>9</b> 0	-1.3	0.5		A	.45E-6	4.6970091	-1.8566921
91				B	.51E-6	6.4463358	-1.8322313
92	-1.4	0.65		в	.53E-6	6.6025901	-1.8171647
93	-1.3	0.5		в	.54E-6	6.4463363	-1.8322287

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No.	b2	b3	n*	Ń	SDSS	P*	U*
94	-1.3	0.4	0.85	в	.69E-6	8.6997929	-1.8698852
95	-1.3	0.6		в	.50E-6	6.1868677	-1.8182068

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Solutions of Equation T for a Square-Well Potential at T\* = 1.6

					··		
No.	b2	b3	n*	N	SDSS	P*	U*
1	0	0	0.60	A	.215E-6	1.8691945	-0.85430503
2				В	•340E-6	1.9605376	-0.85032463
3	0	-0.25		A	.135E-6	1.8252692	-0.85627973
4				в	.175E-6	1.9074475	-0.85240221
5	-0.5	0		A	.148E-6	1.7977179	-0.84841144
6				В	.183E-6	1.8596156	-0.84428263
7	-0.5	-0.25		A	.270E-6	1.7519943	-0.84980106
8				В	.446E-6	1.8039701	-0.84571457
9	-1.0	-0.25		A	.482E-7	1.6121860	-0.84650528
10				в	.171E-6	1.6306120	-0.84231210
11	-1.0	-0.5		A	.755E-7	1.5492582	-0.84786713
12				в	.166E-6	1.5557830	-0.84367490
13	-1.0	-0.7		A	.111E-6	1.4936109	-0.84903753
14				В	.204E-6	1.4903784	-0.84484112
15	-1.3	-0.4		A	.135E-6	1.4310071	-0.84696090
16				В	.175E-6	1.4172444	-0.84270728
17	-1.3	-0.15		A	.111E-6	1.5106111	-0.84543145
18				в	.264E-6	1.5102673	-0.84120393
19	-1.5	0		A	.148E-6	1.4485084	-0.84489596
20				в	.183E-6	1.4383991	-0.84067762
21	0	0	0.80	A	.222E-6	4.6746984	-1.4074190
22				B	.423E-6	5.0253215	-1.3958354

		~					
No.	b2	b3	n*	N	SDSS	P*	U*
23	0	-0.25		A	.230E-6	3.9631839	-1.4211581
24				В	.340E-6	3.9980166	-1.4105668
25	-0.3	0		A	.270E-6	4.0540509	-1.4031007
26				В	.446E-6	4.1982503	-1.3909540
27	-0.3	0.25		A	.230E-6	4.6901641	-1.3925028
28				в	.550E-6	5.1130581	-1.3797793
29	-0.5	0.1		A	.354E-6	3.8538678	-1.4000428
30				в	.660E-6	3.9859405	-1.3876967
31	-0.5	0.4		A	.229E-6	4.6834607	-1.3864090
32				В	.512E-6	5.1583395	-1.3732843
33	-0.8	0.25	0.80	A	.347E-6	3.5820916	-1.4015365
34				в	.591E-6	3.7896557	-1.3897009
35	-0.8	0.55		A	.241E-6	4.5673337	-1.3823862
36				В	.333E-6	5.1012182	-1.3689859
37	-1.0	0.7		A	.113E-6	4.6176586	-1.3791394
38				В	.352E-6	5.2640147	-1.3655047
39	-1.94	0.96	0.60	A	.847E-7	1.5097176	-0.84078944
40				в	.144E-6	1.5166358	-0.83673191
41			0.80	A	.496E-6	5.3855863	-1.4054890
42				В	.438E-6	7.6563807	-1.3905199
43	-1.9	0.7	0.60	A	.622E-7	1.4449277	-0.84229720
44				в	.146E-6	1.4388801	-0.83823323
45			0.80	A	.153E-6	7.4341240	-1.4802871
46				B	.542E-6	11.305983	-1.463501

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No.	b2	b3	n*	N	SDSS	P*	Ű*
47	-0.5	0.25	0.60	В	.187E-6	1.9120777	-0.84293973
48	-1.0	0.25		B	.257E-6	1.7625946	-0.83983338
49	-1.8	0.55	0.80	B	.654E-6	15.248972	-1.5510526
50	-0.5	0.5	0.60	B	.149E-6	1.9617392	-0.84167314
51	-1.0	0.5		B	.189E-6	1.8216939	-0.83869648
52	-1.0	0		В	.199E-6	1.6991723	-0.84103537
53	-1.5	0.25		В	.218E-6	1.5318680	-0.83917749
54	-1.5	0.5		B	.182E-6	1.6143057	-0.83782256
55	0	0.5		в	.144E-6	2.0571389	-0.84674716
56	-1.9	0.8	0.80	A	.254E-6	6.0166392	-1.4359179
57				в	.457E-6	8.9587574	-1.4207580
58	-1.8	0.7		A	.288E-6	6.1483250	-1.4508893
59				B	.390E-6	9.2330332	-1.4364240
60	-1.7	0.5		A	.349E-6	9.9461813	-1.5726101
61				B	.544E-6	14.911380	-1.5547526
62	-1.8	0.55		A	.327E-6	10.196666	-1.5700102
63				В	.668E-6	15.248972	-1.5510523
64	-1.7	0.5		A	.358E-6	9.9461727	-1.5726089
65				B	.568E-6	14.911425	-1.5547485

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T	AR	T.E	8
			<b>v</b>

No.	b2	b3	<b>n</b> *	N	SDSS	p*	U*
1	0	0	0.65	A	.117E-6	2.9417796	-0.43090212
2				В	.109E-6	3.0596471	-0.42948377
3	0	0.25		A	.126E-6	3.0865679	-0.42920959
4				B	.182E-6	3.2427082	-0.42774475
5	0	-0.25		A	.119E-6	2.7591805	-0.43298745
6				в	.176E-6	2.8308783	-0.43160701
7	-0.5	0		A	.158E-6	2.4683772	-0.43806720
8				в	.202E-6	2.5026784	-0.43693936
9	-0.5	0.25		A	.104E-6	2.7385952	-0.43410254
10				В	.200E-6	2.8348296	-0.43284488
11	-0.8	0.4		A	.121E-6	2.5877671	-0.43796778
12				B	.202E-6	2.6753817	-0.43701184
13	0	-0.3		A	.105E-6	2.7158422	-0.43347657
14				B	.156E-6	2.7769718	-0.43210042
15	-0.8	0.5		A	.150E-6	2.6908870	-0.43619907
16				в	.218E-6	2.8010728	-0.43514991
17	0	0	0.85	A	.192E-6	6.2781415	-0.82360291
18				B	.505E-6	6.7088246	-0.81408644
19	0	0.25		A	.314E-6	7.1942997	-0.81413543
20				В	.523E-6	8.0834370	-0.80403733
21	-0.5	0.25		A	.437E-6	6.3356385	-0.81860006
22				в	.501E-6	7.1070642	-0.80737972

Solutions of Equation T for a Square-Well Potential at  $T^* = 2.2$ 

No.	b2	b3	n*	N	SDSS	<b>p</b> *	U*
23	-0.5	0.15		A	.335E-6	5.6297345	-0.82832789
24				в	.680E-6	6.1704793	-0.81750095
25	-0.3	0.15		A	.237E-6	6.2571015	-0.81949794
26				в	.543E-6	6.8481293	-0.80884945
27	-0.3	0.1		A	.318E-6	5.9249916	-0.82297838
28				₿	.580E-6	6.3768787	-0.81246257
29	-0.6	0.25		A	.356E-6	6.1428475	-0.82267737
30				в	.434E-6	6.9519725	-0.81133401
31	-0.517	0.208	0.65	A	.644E-7	2.6842237	-0.43494928
32				B	.188E-6	2.7690258	-0.43372631
33			0.85	A	.330E-6	6.0534577	-0.82257223
34				B	.688E-6	6.7438269	-0.81145108
35			0.001	A	0	0.99923414	0.99762475
36				в	0	0.99923420	0.99762601
37			0.01	A	0	0.99254209	0.97631854
38				в	0	0.99254429	0.97633207
39			0.10	A	.722E-8	0.94775707	0.77018553
40				в	.136E-7	0.94805825	0.77045906
41			0.20	A	.111E-7	0.95598066	0.55318999
42				в	.146E-7	0.95762551	0.55392814
43			0.30	A	.245E-7	1.0473721	0.34096867
44				в	.381E-7	1.0525357	0.34204674
45			0.50	A	.705E-7	1.6375816	-0.09676384
46				в	.103E-6	1.6661731	-0.09591829

No. b <sub>2</sub>	b3	n*	N	SDSS	P*	Ü*
47	<u> </u>	0.60	A	.112E-6	2.2548254	-0.32303154
48			В	.161E-6	2.3131950	-0.32219064
49		0.80	A	-284E-6	4.8495140	-0.74019480
50			в	.450E-6	5.2332501	-0.73362398

## APPENDIX C

# COMPUTER PROGRAM

This appendix gives a listing of the computer program that was used to compute the thermodynamic functions of a square-well potential using perturbation theory.

```
PRINT 'SWPT.BAS-THIS PROGRAM COMPUTES THE THERMODYNAMIC FUNCTIONS'
FRINT 'FOR A SQUARE-WELL LIQUID USING PERTURBATION THEORY.'
DIM UR(20),F(20,30),FR(20,30),G(20),FF(20,30),P(20,30),U(20,30)
REM ENTER UR(REF INT ENER), T1(REF TEMP), A1,...,A6(PADE COEF
10
20
30
40
50
        REM FOR P REF)
        FOR I = 1 TO 19
60
70
80
        READ UR(I)
        NEXT I
        DATA 0.99762601.0.97633207..883..770..661..554..449..345..239..131
        DATA .019+-.096+-.212+-.326+-.434+-.537+-.634+-.725+-.812
READ T1
90
100
110
120
        DATA 2.2
130
        READ A1+A2+A3+A4+A5+A6
140
        DATA -2.33567,4.22295,-1.90424,-1.56833,.796711,-.178773
150
        REM CALCULATION OF F(0.001)TSTAR)
160
        FOR J = 1 TD 30
T2 = .65 + J#.05
F(1,J) = LOG(20/T2) - 3.316125579*.001*(EXF(1/T2) - EXF(1/20))
180
190
        NEXT
200
        REM CALCULATION OF FR(.001.TSTAR)
210
        FOR J = 1 TO 30
        \begin{array}{l} 12 = .65 + J \star .05 \\ FR(1,J) = F(1,J) - (1 - (T1/T2)) \star (1 - UR(1)) \end{array}
220
230
        NEXT J
240
        REM CALCULATION OF FR(NSTAR) TSTAR)
PRINT "TYPE THE NO OF INT PTS"
250
260
270
        INFUT N1
        280
290
300
310
320
330
        G(1) = FNX1(.001)
340
350
        G(2) = FNX1(.01)
        G(3) = FNX1(.05)
360
        G(4) = FNX1(.1)
370
        Fok I = 5 TO 19
X0 = (I - 3)*.05
Fok J = 1 TO N1
X = X0 + (J - 1)*D
380
390
400
410
        S = S + FNX2(X)/X
420
430
        NEXT J
S = S - .5*((FNX2(X0)/X0) + FNX2(X0+.05)/(X0+.05))
440
450
        S = (2*S*E)/3
460
        G(I) = G(I - 1) + S
        S = O
NEXT I
470
480
496
        FOR J = 1 TO 30
FOR I = 1 TO 19
500
510
        FR(I_{J}) = G(I) + FR(1_{J})
520
        NEXT I
530
        NEXT J
540
        REM CALCULATION OF FP(NSTAR+TSTAR)
        FOR J = 1 TO 30
FOR I = 1 TO 19
T2 = .65 + J*.05
FF(1,J) = (1 - T1/T2)*(1 - UR(I))
550
560
570
580
590
        NEXT I
600
        NEXT J
        FOR J = 1 TO 30
FOR I = 1 TO 19
610
620
630
        F(I_{J}J) = FR(I_{J}J) + FP(I_{J}J)
640
650
        NEXT I
660
        NEXT J
        REM CALCULATION OF P(NSTAR+TSTAR)
670
680
        DN = .05
        DT = .05
CN = 1/(12*DN)
CT = 1/(12*DT)
FOR J = 1 TO 30
690
700
710
720
        F(3,J) = 1.5#.05#CN#(-25#F(3,J)+48#F(4,J)-36#F(5,J)+16#F(6,J)-3#F(7,J)
F(4,J) = 1.5#.1#CN#(-3#F(3,J)-10#F(4,J)+18#F(5,J)-6#F(6,J)+F(7,J))
730
740
        FOR I = 5 TO 17
D = (I - 2)*.05
750
760
        P(I,J) = 1.5*D*CN*(F(I-2,J)-8*F(I-1,J)+8*F(I+1,J)-F(I+2,J))
770
780
        NEXT I
```

790 P(18,J) = 1.5\*.8\*CN\*(-F(15,J)+6\*F(16,J)-18\*F(17,J)+10\*F(18,J)+3\*F(19,J)) BOO F(19,J) = 1.5\*.85\*CN\*(3\*F(15,J)-16\*F(16,J)+36\*F(17,J)-48\*F(18,J)+25\*F(19,J)) 810 NEXT J REM CALCULATION OF U(NSTAR, TSTAR) FOR I = 3 TO 19 820 830 840 U(1+1) = -.7\*CT\*(-25\*F(I+1)+48\*F(I+2)-36\*F(I+3)+16\*F(I+4)-3\*F(I+5)) U(1+2) = -.75\*CT\*(-3\*F(1+1)-10\*F(1+2)+18\*F(1+3)-6\*F(1+4)+F(1+5)) 850 FOR J = 3 TO 28 860 T2 = .65 + J#.05 U(I,J) = -T2\*CT\*(F(I,J-2)~8\*F(I,J-1)+8\*F(I,J+1)-F(I,J+2)) 870 880 890 NEXT J U(1,29) = -2.1\*CT\*(-F(1,26)+6\*F(1,27)-18\*F(1,28)+10\*F(1,29)+3\*F(1,30)) 900 U(1,30) = -2.15\*CT\*(3\*F(1,26)-16\*F(1,27)+36\*F(1,28)-48\*F(1,29)+25\*F(1,30)) 910 920 NEXT I MEAL 1 REM FRINT OUT OF N\*\*F\*\*F\*\*U\* FUK J = 1 TO 30 T2 = .65 + J\*.05 FRINT FRINT \*TSTAR = \*\$T2 FRINT \*N-STAR',\*F-STAR',\*P-STAR',\*U-STAR\* 930 940 950 960 970 980 FOR I = 3 TO 19 D = (I - 2)\*.05 PRINT D;F(I;J);P(I;J);U(I;J) 990 1000 1010 1020 NEXT I 1030 NEXT J NEAT J REM PRINT OUT OF N\*,S\*,H\*,G\* FOR J = 1 TO 30 T2 = .45 + J\*.05 PRINT 1040 1050 1060 1070 FRINT \*T-STAR =\*;T2 FRINT \*N-STAR\*;\*S-STAR\*;\*H-STAR\*;\*G-STAR\* FOR I = 3 TO 19 I = (I - 2)\*.05 1080 1090 1100 1110 FRINT D+U(I+J)-F(I+J)+U(I+J)+2\*F(I+J)/3+F(I+J)+2\*F(I+J)/3 1120 1130 NEXT I 1140 NEXT J 1150 END

#### APPENDIX D

## RESULTS OF THERMODYNAMIC FUNCTIONS

The following notations are used:

T	STAR	Value of the reduced temperature.
N	STAR	Value of the reduced density.
F	STAR	Value of the reduced Helmholtz free
		energy.
P	STAR	Value of the reduced pressure.
U	STAR	Value of the reduced internal
		energy.
H	STAR	Value of the reduced enthalpy.
G	STAR	Value of the Gibbs free energy.

TSTAR =	•7					
N-STAR		F-STAR	P-STAR		H-STAR	
.05		5.6813	.516795		. 620039	
•1		5.88169	.26022		.265046	
.15		5,9035	111926		- 774673F-	01
.2		5.85621	407954		413601	VI
•25		5.77593	682714		743477	
.3		5.67702	947035		-1 07077	
.35		5.5473	+/0//33		-1.0/022	
.4		5.43774	-1 55005		-1+40331	
. 45		5 70744	-1+33873		-1+/4200	
• <b>••</b> ••		5.14507	-1+80003/		-2.09448	
.5 .55		5 07014			-2+40081	
• 4		J.VQVIG	-2+14811		-2.82026	
+0		4+70001	-1.98812		-3.17844	
+0J		4+81137	-1.6372		-3.51777	
+/		4.74194	-1.12647		-3,84136	
+/3		4./06/1	350649		-4.1461	
•8		4.71298	<b>•699812</b>		-4.43197	
•85		4+76693	2.03008		-4.70533	
	-					
JSIAK =	+/5					
N-5IAK		F-SIAR	F-STAR		U-STAR	
+05		5+63758	•5533		•646983	
•1		5.86165	•32968		•315476	
•15		5,9063	102523E-0	)1	-+427485E-	02
•2		5.88143	274804		318174	
•25		5.82314	519024		626207	
•3		5.74602	770406		931312	
•35		5.65351	-1.02645		-1.24226	
• 4		5.55159	-1.28259		-1.55908	
•45		5.44075	-1.53362		-1.88764	
•5		5.32648	-1.7067		-2.22501	
.55		5,21587	-1.74852		-2.56531	
+6		5,11791	-1.56855		-2.89974	
•65		5.04381	-1.20616		-3.21656	
•7		4.99575	686107		-3.51871	
•75		4,98084	.9170925~0		-3.80329	
•8		5.00618	1.14497	-	-4.07025	
.85		5.07835	2.40040		-4.30547	
100		010/000	2.4/04/			
TSTAR =	•8					
N-STAR	• -	E-STAR	P-STAR		HECTAR	
•05		5.59504	505747		470707	
. 1		5.0700E	+ 303277		+0/0323	
.15		5 00000	+37V433 707004E.0		+337388	~ 4
. 7		5 00077	+/8/V70L-V	1	+3786285-	01
• 2		J+07744 E 0/010	138293		-+2343/	
ديني. ۳		5.00017	-+3/3/7		523101	
•3		J+8V214 5 700A/	-+37/368		809085	
•30 ▲		J+/27V8	820809		-1.10057	
+ <del>4</del> AE		3+64674	-1.040//		-1.39755	
+ 40 E		2+22663	-1.25209		-1.70553	
+ J E#		0+46344	-1,38793		-2.02176	
•33		3.3/41	-1.39887		-2.34074	
+0		5.29/04	-1,20143		-2.65422	
• 6 3		5+24274	829006		-2.9512	
•7		5.21356	300774		-3.23443	
•75		5.21644	•478788		-3.50117	
•8		5,25846	1.53423		-3,7514	
•85		5.34659	2.89331		-3,99063	

TSTAR =	•85			
N-STAR		F-STAR	P-STAR	U-STAR
•05		5.5538	.613434	+690675
•1		5.81686	<b>•444078</b>	.398219
•15		5.89913	•157205	.11612
•2		5.91118	554955E-01	160809
•25		5.88914	249414	432566
.3		5.84791	445063	701721
•35		5.79198	639346	976066
•4		5.72732	827395	-1.25558
.45		5.65513	-1.00368	-1.54545
45		5.58055	-1.10666	-1.84308
•55		5.50997	-1.09037	-2.1433
		5.45135	- 877489	-7.47974
.65		5.41453	496211	
•7		5.40201	-392032F-01	-7.98444
.75		5.42057	.820301	-7.77540
.8		5.47770	1.07707	-3+23347 -7 471
.85		5.57052	7 24075	-3+7/1
•03		J+J/7J2	3+240/J	-3:0701/
TSTAR =	•9			
N-STAR		F-STAR	P-STAR	U-STAR
•05		5.5138	.638489	<b>↓7086</b> 2
•1		5.79312	. 491745	.437399
.15		5.89105	.226981	.16597?
.2		5.9185	.035888	0557005-01
25		5.01155	137078	- 750770
.3		5.88527	309505	- XAXAO
. 35		5.04450	- 47905	- 045540
. 4		5 70544		-+ + 000040 -+ + 0057
.45		J+/7J40 5.77077	- 707071	-1 A077
• • •		J+/373/	-+/020/1	-1.4033
• J		J+00133	-+60664/	-1+0844
• 3 3		J+02/42 5 5050	-•810148	-1+70/94
•0		J+J0J2 E E/70	387348	-2+2400
*65		3.3037	200395	~2+51059
*/		3+30019	• 341420	-2+/6236
•/5		5.578/1	1.12389	-2,99947
•8		5.66854	2.18323	-3,22191
•85		5.78325	3.5647	-3.43456
TSTAR =	. 95			
N-STAR	•70	F-STAR	P-STAP	U-STAR
.05		5.47505	. 440911	
.1		5.74001	574707	*/27393
.15		5.00007	+ 337373	+4020// 310/E/
.2		5 00007	117444	+210400
.25		J1722V/ 5 930/7	+11/040	- 3731236-01
.7		J+72003 5 01574	- 100017	- FO17
.75		J+71J/4 5 000/0	- 77777	
		J+00007	-+333/3	-+/00//0
• <del>4</del> • E		5.83346	-+46804/	-1.0168/
**3		5.811/8	383303	-1.2/624
+J 62		2.10823	632746	-1.34234
•22		5.72955	570781	-1.81116
•0		5.70199	331922	-2.07516
• 0 0		3.67457	•642786E-01	-2.32525
•/		5.71013	.611824	-2.56377
•75		5.75513	1.3955	-2,78839
•8		5.83667	2.45649	-2.99912
•85		5.96257	3.84741	-3.20058

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TSTAR =	1		
N-STAR	F-STAR	P-STAR	U-STAR
•05	5.43752	+68108	.738806
•1	5.74446	•57278	•490224
.15	5.86904	.345596	.250427
•2	5.92264	191228	.150331F-01
•25	5.94135	▲538957E-01	215963
.3	5.9405	7905345-01	444755
.35	5,92572	203839	477958
.4	5,903	315319	915540
.45	5,87429	- 407499	-1 14104
.5	5,84474	- 471400	-1+10174
.55	5,91991	-++31022 - 740055	-1 474
. 4	5+01001		-1.07012 ~
+0	J+0/473	10004/	-1+92092
*03	J+8V736 F 87769	• 302488	-2.15852
+/	3.63/02	•822186	-2+38511
•/5	3+87325	1.63996	-2.59851
•8	5+98532	2.70242	-2,79869
•82	6+1213	4.10179	-2,99009
TOTAD -	1 05		
N-STHK	FTOLAR	r-Siak	U-STAR
•05	5.40116	•699337	•751658
•1	5./1993	•607508	•514893
+15	5.85593	• 396433	·286522
•2	5.92074	+257807	•623304E-01
•25	5.95046	.135741	157668
•3	5.9605	197099E-01	375564
•35	5,95683	863279E-01	597648
• 4	5.94542	177137	823929
• 45	5.92844	246618	-1.05859
•5	5,91055	247466	-1.29954
•55	5.89716	150166	-1.54259
•6	5+89474	.109736	-1.78144
• 65	5,91116	.518007	-2.00771
.7	5.94942	1.07537	-2,22352
.75	6.01581	1.86113	-2.42676
.8	4.11742	7 07405	-7 41747
.85	4.24251	A. 779	-2.01/92
	0+20201	4(332	-2*/77/1
TSTAR =	1.1		
N-STAR	E-STAR	R-STAR	HARTAR
.05	5,36592	. 715974	.747979
.1	5.69546	470070	+/032/0
.15	5.84194	+037077	+J3/207 740077
.2	5.01407	+442040 740771	+3172/3
9E	5 05/55	•318331	+103281
+23	0+70600	•210146	-+104/16
*3	J+7/6J E 80000	•109492	312/13
• 30	J+78292	•2050/4E-01	524/
+ 4	5.981/9	515156E-01	7407
•40	5+7/547	100372	9647
• 7	3.76822	838661E-01	-1.19469
• 55	5.96621	•031468	-1.42669
•6	5+97465	.300446	-1.65469
• 65	6.00135	•71393	-1.87068
•7	6.04942	1.27554	-2.07668
•75	6+12505	2.06222	-2.27068
•8	6+23532	3.12724	-2.45268
•85	6.3887	4.54127	-2.62667

ί,
TSTAR =	1.15		
N-STAR	F-STAR	P-STAR	U-STAR
.05	5.33175	.731089	.773828
.1	5.67112	.667904	1557662
•15	5.82698	484842	.349144
.2	5.91128	.373591	.144448
.25	5,96012	278081	5441455-01
.3	5,98912	. 191477	- 955775
.35	4.00475	110047	- AED1E
. 4	4.01707	+120047	- 443013
45	6.01302	-831804E-01	-+004/37
+ 40	0+VI04J 4 01050	• 331618E-01	8/9009
•J 55	0+V1752 4 00704	+0/3240E-V1	-1.099
+00	0.02/20	•19/306	-1.32092
+0 / E	6.04561	•47458	-1.539
+60	6.081/1	+872831	-1.74561
+/	6+13873	1.4583	-1,94265
+75	6.22279	2.2458	-2.12821
•8	6.34098	3.31194	-2.3023
•85	6,50192	4.73232	-2.46873
TSTAR =	1.2		
N-STAR	F-STAR	F-STAR	U-STAR
•05	5,29861	•744979	• <b>783</b> 487
•1	5.64698	•694327	•576326
.15	5.81153	•523522	.37649
.2	5,90436	.424248	.180341
•25	5.96158	.340354	012166
•3	5,99886	.266618	202826
+35	6.02295	•207465	39716
•4	6.03982	.168317	595171
.45	6.05218	.155561	- 80049
<b>•</b> 5	6.06441	,205927	-1.01172
.55	6.0814	. 749724	-1.00700
.6	6.10884	. 4342024	-1.47000
. 45	4.15755	1 05400	-1 /7000
.7	4.91970	1 + VJODZ 1 27507	-1.010077
.75	4.31057	1+02J02 2 A1AAO	
.9	6+31037 4 A7401	2+41407	-1+77/00
•0 0E	0+43601	3+48124	-2+16449
•85	6.60387	4.90/45	-2.32396
TOTAD -	1 25		
N-CTAD			
.05	F DAAAE	F-51AK	U-SIAK
+VJ	₩÷40040 5 /074	•/3//47	•79236
• L	J.0231 E 70545	•/1864	.593483
+15	3./7363	.559106	.401645
•2	5.87632	•47085	•213329
+25	5.96124	• 397648	•285308E-01
• 3	6+00615	•335754	154507
• చె	6+03801	•289729	341069
•4	6+0628	•265042	531138
• 45	6.08337	•268175	-,728265
•5	6.10404	•33343	930669
•55	6.12953	<b>•489178</b>	-1.13482
•6	6.16534	.781054	-1.33546
•65	6.21796	1.20768	-1.52553
•7	6.29075	1.77996	-1.70681
•75	6.38965	2.56892	-1.87754
•8	6.52177	3.63697	-2.03769
•85	6+69602	5.06853	-2.1908

TSTAR =	1.3		
N-STAR	F-STAR	P-STAR	U-STAR
.05	5,23521	•769552	.800514
.1	5.59951	•741077	.607288
.15	5.77944	.591954	•424827
•2	5.88735	•513868	.243744
•25	5.95938	.450529	.660594E-01
.3	6.01133	.399574	109937
.35	6.05036	.365659	289323
.4	6.08247	.354307	- 472085
.45	6.11062	. 777170	- 441477
.5	6.13907	.451177	- 954245
.55	6.17242	. 418074	-1.050255
	A. 2158A	.014402	-1 24547
. 65	6.27587	1.74404	-1.27077
.7	A. 35543	1.00004	-1.40254
.75	6, 64111	1074227 0 71107	
.0	4.50070	20077	-1 92049
.95	2+37730 2,77050	34/60// 5 31777	
+03	0+//7J2	3+21/3/	-2.00/93
TSTAR =	1.35		
N-STAR	F-STAR	P-STAR	H-STAR
.05	5.20485	. 780447	808047
.1	5,57424	.741050	4070047
.15	5.743	•/01037	+0237V4 . AA4747
. 7	5 07740	+ 022J/ 557/00	+770203
.75	J+0//04 5 05407	4 333677	•2/1706
. 7	J+7J023 4 A1A40	+47747/ AFD//A	•10079
.5		+ 438004	0808/1E-V1
•20		+4337/1	241421
**	Q+V7720 ∠ 17440	•43677/	-+41/429
•47	0+13442	• 468382	
+J 85		+560112	/8/33/
• 33	0+21V/ 4 0/17/	•/3/809	
+0	0 • 20003 0 • 20003	1.04212	-1.1621/
• 6 0	6+32807	1.4/589	-1.3381/
+ /	6+41428	2.05396	-1.50601
•/5	6+52583	2.84416	-1.66408
•8	6.66981	3.9139	-1.81238
•85	6.85541	5.35504	-1.95416
TOTAD -	1 .		
N-STAR	III F-STAR	P-CTAD	II_CTAD
.05	5,17534	.700400	.915044
.1	5,5577	701157	. 477447
.15	5.7444	4/01100	+03/403
	5.84725	+037015	+700177
.25	5,05107	+J7000J 5//040	17704
.7	4.01449	+ 344780	+13304
.35	4.04834	-501254	
+30	4 1175	+JV12JO E4777	
• 7	Z 18510	+JI3// EE7764	- 540447
•~~~ _5	ロ+1JJ17 人、407時間	+33//30	
	2+27/JJ 2+27/JJ	+001312	-+/200/4 _ 0/61/7
ۍ د ۲	0+24471 2 70334	+ 0488V6 1 + 50/7	-+70300/
•0 45	0+3V221 4 7750	T+1380/	~1.V0481
• 0 3		1+37361	-1.23431
•/	6+46/41	2+17628	-1.41637
•/2	0.08461	2+96704	-1.5688
• 8	6./3388	4.0375	-1.71179
+ 20	6+72404	5.48293	-1.8485

à

TSTAR =	1.45		
N-STAR	F-STAR	P-STAR	U-STAR
•05	5.14662	•800057	<b>821523</b>
•1	5.53071	•799111	.650074
•15	5.72971	•676905	•484701
•2	5.85637	<b>•625125</b>	.322352
•25	5.94677	•587298	•163049
•3	6.01693	•564614	•526166E-02
• 35	6.07452	.562041	15557
•4	6.12553	•585238	319426
•45	6.1733	•640965	• 489363
•5	6.22188	•755531	663841
•55	6.27553	•952146	839842
•6	6.33901	1.26717	-1.0128
.65	6.41785	1.70709	-1.17666
•7	6.51564	2.29017	-1.33294
•75	6.6381	3.08144	-1.48011
•8	6.7923	4.1526	-1.61819
•85	6.98768	5.60199	-1.75017
TOTAR	. <b>-</b>		
N-STAR =	1+J E-STAD	D-CTAD	
N-STAK		F-SIAK	U-SIAR
•00	5,1186/	+808867	•827565
*15	J.JV84/ 5 71000	+815877	•661849
• 1 7	J•/1277 E 04E4E	+/01446	•501963
* A 195	J+843V3 E 04033	•63/263	.34505
• 2 J		+020811	•191048
*3	6+V1018 4 07014	+ D12273 (+ D775	+385034E-01
• GG ·	4 17541	+010//0	
. 45	A.19904	+001702 719400	
.5	6.94744	+/100%0 DA74/F	-+437032
,55 ,55	6+24344 4.30304	1 040400	- 770400
•00	4.3722	1.74045	- 045494
. 45	6.0722 6.4545	1.0040	-1.10407
.7	2,5505	2.39447	-1.25509
.75	A . 48484	7,19977	-1.20007
.9	4 94547	3+10022	-1 57/33
.85	7.04545	4+20VV3 5.71700	-1.45043
100	7 + 0 + 0 + 0	2.11200	-1+00043
TSTAR =	1.55		
N-STAR	F-STAR	P-STAR	U-STAR
•05	5.09144	•817111	•833233
+1	5.48659	<b>•831562</b>	•672844
•15	5.69626	.724405	،51813
+2	5.83339	•687331	•366272
•25	5.93407	+663775	•217227
•3	6.01441	•6569	.696193E-01
• 35	6.08238	•671844	808388E-01
•4	6.14396	•714356	234133
+45	6.20269	•791284	393089
+5	6.26253	•92573	-,556321
•55	6+32754	1.13883	720958
+ 0 	6+40217	1.46319	882776
+0U 	0+47138	1+70847	-1.03606
+ / 75	6+37946	2+4757	-1.18226
+/3	0+/3141	3+2881	-1.31993
•0 .85	0+074J2 7.000A1	7+30V32 5 0174/	-1 53053 _1 53053
• • •	/ + V 7 0 4 1	2+01/00	-1+3/23/

TSTAR =	1.6		
N-STAR	F-STAR	P-STAR	U-STAR
•05	5.0649	.824837	•838523
<b>1</b>	5.46506	.846268	.683151
.15	5.67957	.745926	•533267
•2	5.82144	.715516	.386155
•25	5,92678	+698428	•241777
•3	6.01173	.698714	•987778E-01
.35	6.0844	.721604	469653F~01
• 4	6.15078	•772857	195477
• 45	6.21447	.859395	
.5	6.27941	1.00285	- 507595
:55	6.34957	1,22342	- 667102
•6	6.42926	1.55202	823845
.65	6.52346	1,99972	- 972341
.7	6.6359	2.58913	-1.11397
.75	6.77216	3,38175	-1.24734
.8	6.9393	A. 45473	-1 77947
.85	7.14705	5 01/5	-1+3/24/
+00	/+14/05	0+7140	-1+49209
TSTAR =	1.65		
N-STAR	F-STAR	P-STAP	U-STAP
.05	5.03902	.832097	. 847484
.1	5.44389	.840079	.497904
.15	5.66294	.744144	.547494
.2	5,80927	741004	+34/400
.25	5,01000	+/71/70 77A00	+ TV TO 74 A01 7
• 2.0	4 00007	+/3070	+204012
• <del></del>	6+00827 4 09574	4/0/774	+12013/
+ 00 A	0+V0J30 / 15/07	+/05041	-+131802E-VI
+4	0+10023 ( 00450	+8~\818	+159183
+ 40	0+22407 4 00470	•7233/6	308515
+0	6+27432	1.0753	461843
• 33	6+36731	1.30289	616511
+0	6+453/5	1.63544	768514
• 60	6.00246	2.08544	912504
• /	6.66717	2.6767	-1.04984
•/5	6.80948	3.46972	-1.17917
•8	6.98042	4.54324	-1.30051
•80	7.1918	6.00604	-1,41651
TSTAR -	1.7		
N-STAP	E-STAD	D-CTAP	U-STAD
. 05	F 01777	67667/	U-SIAR DADIE1
- 1	5 40707	+030730	•848131
+1		+8/30//	.701913
+12	J+6464	+/851/5	• 560855
+ 2 05	J+/7672 E 0107/	•/66918	•4223/9
ن <u>کے</u> ہ	3+710/6	+/61616	•286507
• 3 . 7 E	6.00412	+7/4966	.151919
+ 30	6.08336	•812331	•147371E-01
+4	6+1604/	•879542	-+125024
• 40	6.23322	•983597	-+26996
•5	6.30747	1.14349	418795
• <del>3</del> 3	6.387	1.37768	568879
+6	6+47591	1+71398	716433
+ 60	6+57885	2.16611	856198
• /	6.67963	2.75912	989482
•75	6+84372	3.55251	-1.11502
•8	7.01823	4.62654	-1.23278
•85	7,23302	6.09222	-1.34537
-			

. .

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TSTAR = N-STAR	1.75 F-STAR	P-STAD	N-STAD
.05	4,98912	. 845774	0-31HK
.1	5.4076	.995778	10J2J42 7105
.15	5.62996	.803110	.577449
.2	5.78444	. 700415	• 37 3 4 6 7
.25	5,90215	+770413	• 4307J7
.3	5,99936	.809827	.176207
.35	6.08452	.853805	.429457E-01
.4	6.16363	.928311	092812
.45	6.24052	1.04038	233625
•5	6.31901	1.20778	378193
.55	6.40284	1.44819	- 524029
• 6	6.49597	1.78802	667333
~65	6.6029	2.24218	- 803106
•7	6.72748	2.83683	- 93259
.75	6.87516	3.63057	-1.05453
•8	7.05304	4.70507	-1.16893
•85	7.27104	6.17351	-1,2783
			212,00
TSTAR =	1.8		11 OTAD
	A QAEAE	FTDIHK OF1A/	0-51AR
+05	4+78JVJ E 78247	+83140	• 800070
+ L - 1 E	J+3824/ 5 41747	•876711	•/185/2
•10	J+01303 5 77105	+820004	+ 383332 AF AF 7 A
• <u>~</u>	5 00707	+012007	• 4343/4
• 20	0+07020 5 00407	+81//84	• 320230
• 3	J+774V/ 4 00704	+842/4/ 000070	•177141 (057475 A1
+33	0.00274	+8727/8	•673/43E-U1
+ 4 	0+10081	•7/43/3	-+624289E-01
+40	0+24002 4 70017	1.074	-+177313
+ J 55	0+32713	1+20847	337861
ن د. ۲	0+41/ 4 E1/11	1.05704	-+481637
+0	0+01411 4 40401	1+83/74	-+620776
+0J	0+02701 4 78799	2+31403	-•/329/3
• /		2+71023	-+8/8868
•/3		3+/0427	79/428
+0		4+//724	-1.10864
+00	/+30010	6.2002	-1.21498
TSTAR =	1.85		
N-STAR	F-STAR	P-STAR	U-STAR
• 05	4.94152	<b>.857219</b>	•860623
•1	5.36268	<b>•9078</b> 62	•72622 <del>9</del>
•15	5.59744	•836093	•596619
•2	5.75919	<b>•833599</b>	•469366
•25	5.88404	•84359	•344498
•3	5,98832	<b>•87389</b>	•220831
• 35	6.08048	•930037	•094781
•4	6.16713	1.01794	- <b>.3365</b> 99E-01
•45	6.25163	1.14473	166835
•5	6.33794	1.32593	303593
•55	6.42965	1.57778	441536
+6	6.53052	1.9241	577109
• 65	6.64479	2.38198	-,705543
• /	6.77637	2.97966	828023
•/5	6.93065	3.77404	943386
•8	7+11471	4.84739	-1.05159
•85 •	7.33862	6,32283	-1.15506

TSTAR = N-STAR +05	1.9 F-STAR 4.91852	P-STAR	U-STAR
•1 •15 •2	5.34321 5.58139 5.74449	•918236 •851278	•733482 •607266
•25	5.87463	•86804	• <b>3</b> 61795
•3	5.98215	•903388	• <b>2</b> 41369
•35	6.07784	•96514	•118649
•4	6.16766	1•05922	-•642196E-02
•45	6.25567	1,19278	136104
•5	6.34558	1,38034	269245
•55	6.44091	1,63747	403577
•6	6.54535	1,98677	535578
•65	6.66301	2•44636	660629
•7	6.79781	3•04543	779887
•75	6.95512	3.84011	892194
•8	7.14203	4.91585	997567
- 85 - 94797	7+36867	6.39154	-1,09829
N-STAR	F-STAR	F-STAR	U-STAR
•1	5.32407 5.54548	•007041 •92808 845485	•88/83/ •740353
•2 •2	5.73376	•872355	•01/300 •496648 370105
•3	5.97563	•93138	•260854
•35		•998445	•141271
•4 •45	6.16749 6.25882	1.09838	•194397E-01
•5	6.35214	1.43196	236681
•55	6.45093		367546
•6	6.55875	2.04622	496156
•65	6.67961	2.50744	617993
・7	6.81747	3.10782	734224
・75	6.97766	3.9028	843643
•8	7.16727	4.97891	946309
•85	7.39649	6.45681	-1.04447
TSTAR =	2		
+05	4.87401	+51AK +872759	0-STAR •871183
•15	5.54973	•73/427 •879372	•746875 •626982
.25	5.96879	•87028 •913272 •95797	• 30728 • 393769
• 35	6.07061	1.03008	•162781
• 4	6.16668		•439723E-01
•45	6.26118	1.28169	792233E-01
•5	6.35774		205727
•55	6•4598	1,74788	33332
•6	6•57084	2,1027	458724
•65	6.69474	2.56546	577512
•7	6.83551	3.16711	690824
•75	6.99844	3.96234	797521
•8	7.19061	5.03884	897613
• 8つ -	7.42229	6,51877	993322

TSTAR =	2.05		
N-STAR	F-STAR	P-STAD	IL-CTAD
.05	A.85744	.077/77	0-31HR 074770
.1	5.00477	+0//433 04/704	•8/4337 757005
.15	57417	*740324	+/33083
.2	5+33413	+07237	•030114
• 2	3+/083	+90/331	•521285
•20	3.84333	• 934232	•408603
• 3	5.9616/	•983262	•296999
• 30	6+06634	1.06018	•183235
•4	6.16531	1.17097	•673183E-01
•45	6.26281	1.32289	-• <b>528787</b> E-01
•5	6.36246	1.52766	176297
•55	6+46762	1.79904	300787
•6	6.58172	2.15642	423106
• 65	6.70853	2.62066	53903
•7	6.85206	3.2235	649559
.75	7.01759	4.01898	753665
•8	7.2122	5.09581	851314
.85	7.44421	4.57770	- 944479
	/ • <del>• • •</del> • • • • • • • • • • • • • • •	0+3///2	-+7440/8
TSTAR =	2.1		
N-STAR	F-STAR	P-STAP	
.05	A 97175	00400E	077A
••••	7+03133 E 2/051	+001000	+8//4
• <b>1</b>	J • 20831	•734/93	• /59009
+15	5.518/	•904791	+644801
• 2	5+6956	•923568	•532709
•25	5.83532	•954193	<b>₊422687</b>
•3	5.95431	1.00735	•313732
•35	6.06169	1.08884	•202722
•4	6.16342	1+20467	•895882E-01
.45	6.26378	1.36213	277777E-01
•5	6.36637	1.57209	148254
•55	6.4745	1.84778	269772
•6	6.59151	2.20759	- 799714
. 45	6.72107	2+2V/3/ 9.27777	
.7	4 84707	2+0/323	-+375341
+/	0+00/23 7 A7504	3+2//2	-+610234
•/3	7.03324	4.07293	-+/118/2
+ D DF	7.23218	5.15007	-+80/168
•80	/+46841	6+63388	898358
TOTAD -	0 15		
	2+13		
N-SIAR	F-STAR	P-STAR	U-STAR
•05	4.81067	•88613	•880223
•1	5.25058	• <b>96</b> 287	• <b>764</b> 608
•15	5.50343	•916611	•653066
•2	5.68294	•939048	•543602
•25	5.82521	•973228	•436216
•3	5.94674	1.03032	.329814
.35	6.0567	1.11617	.221279
•4	6.16106	1.23681	110776
.45	6.26415	1.39954	382741F-02
•5	6.36954	1.41445	-,1215AQ
155	6.4805	1.80474	
	L. 2000	4+07744 9 95170	- 781030
.45	0+0VV27 2 777A0	2+23030 7 7977*	-+3300/Y
• 2 3	0+/J240 1 00115	2 + / 2334 7 700 A f	-+40/32/ - 5300
*/	0+00110 7 AF(E0	3+52841	-+3/28
•/5	/+03152	4+12437	672039
•8	/+25068	5,20184	765209
▲ HET		A. 49775	Q5A115

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T-STAR = .7			
N-STAR	S-STAR	H-STAR	G-STAR
•05	-5.06126	964568	6.02583
•1	-5.61664	•438526	6.05517
.15	-5.98097	152085	5.82888
•2	-6.26981	68557	5.58424
•25	-6.51941	-1.19862	5.32079
.3	-6.74724	-1.71551	5.03173
.35	-6.96561	-2.24431	4.7213
• 4	-7,1804	-2.78195	4.39845
•45	-7.39792	-3.33139	4.06652
•5	-7.62088	-3.83649	3.7844
.55	-7.85042	-4.25233	3.59809
•6	-8.08675	-4.50385	3.5829
•65	-8.32936	-4.60923	3.72012
•7	-8.5833	-4.59234	3.99096
•75	-8.85281	-4.37986	4.47294
•8	-9.14496	-3.96543	5.17952
•85	-9.47226	-3.35195	6.12031
T-STAR = .75			
N-STAR	S-STAR	H-STAR	G-STAR
•05	-4.99059	1.01585	6.00644
•1	-5.54617	•535263	6.08143
.15	-5,91057	111097E-01	5.89946
•2	-6.1996	501377	5.69822
•25	-6,44935	972223	5.47713
•3	-6.67734	-1.44492	5.23242
•35	-6.89577	-1,92656	4.96921
• 4	-7,11067	-2.41414	4.69653
<b>₊45</b>	-7.32838	-2.91005	4.41833
•5	-7.55149	-3.36281	4.18868
•55	-7,78118	-3,73099	4.05019
•6	-8.01764	-3.94544	4.07221
•65	-8.26037	-4.02067	4.23971
•7	-8.51446	-3.97612	4.53834
•75	-8,78413	-3,74216	5.04198
•8	-9.07643	-3,30703	5.7694
•85	-9.40383	-2,66514	6.73868
1-51AK = +8	0 0745		
NTSTAK	5-51AK	H-SIAK	6-51AK
1	-4+724/4	1.06049	0.78022
4 E	-J.48V28	•01989	6+10015
+13	-3.84462	•112336	5.75675
*# 25	-4 70720	-+3377	5./9369
فينية 7	-4 41122		J+6V700
.75			J+4V3/0 E 4040/
• 30 . A	-7.04448	-2.09179	J+10100
.45	-7.24214	-2.54024	A 7010
.5	-7.4852	-2.07020	7+/617 <u>A</u> ,5701/
.55	-7.71484	-3.97333	A. AA151
.6	-7.95124	-3.45517	4, AQAAQ
.65	-8.19395	-3.50387	4.49007
•7	-8.44799	-3.43495	5.01305
•75	-8,7176	-3,19199	5.57547
•8	-7.00984	-2.72858	6,28128
.85	-9.33722	-2.06176	7.27546

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T-STAR = .	85		
N-STAR	S-STAR	H-STAR	6-97AP
.05	-4.86312	1.09947	5.04075
•1	-5.41865	. 494371	4.11707
.15	-5,78301	.220924	6.00797
•2	-6.07199	- 197806	5.87419
.25	-6.3217		5.70084
•3	-6.54963	99843	5.5512
.35	-6.76804	-1.4023	5.36574
•4	-6,9829	-1.80718	5,17572
.45	-7.20058	-2.21457	4.98601
•5	~7.42363	-2.58085	4.84278
•55	-7.65327	-2.87021	4.78306
• 6	-7.88969	-3.02333	4.86636
.65	-8,13239	-3.04867	5.08372
•7	-8.38645	-2.95831	5.42814
<b>₁75</b>	-8.65606	-2.68862	5.96744
•8	-8.94831	-2.21912	6.72919
•85	-9.27568	-1.53033	7.74535
			/ // 4000
T-STAR = .	9		
N-STAR	S-STAR	H-STAR	G-STAR
•05	-4.80518	1.13428	5.93946
• 1	-5,36072	.760229	6.12095
•15	-5,72508	•317292	6.04237
•2	-6,01407	716536E-01	5.94242
.25	-6.26378	-+443624	5.82016
•3	-6.49172	812786	5.67893
•35	-6.71013	-1,18425	5.52588
• 4	-6.92499	-1.55469	5.37029
•45	-7。14267	-1.92521	5.21746
•5	-7.36573	-2.2555	5.11023
•55	-7,59537	-2.51204	5.08332
•6	-7.8318	-2+63964	5.19216
•65	-8,07449	-2.64418	5.4303i
•7	-8,32855	-2.53474	5.79381
•75	-8,59818	-2.25021	6.34797
•8	-8.89044	-1.76642	7.12402
•85	-9.21781	-1.0581	8.15971
-	<b></b>		
1-51AK = .			
N-STAR	S-SIAR	H-STAR	G-STAR
+00	-4./5051	1.16515	5.91566
+ L + E <sup>2</sup>	-3,30603	.819139	6.12517
+13	-5+6/041	•403395	6.07381
• 4	~3.73737 / Coor	•411183E-01	6.00051
* 20 7	-6+2071	304839	5.90426
+3	-0+43/V4 -/ 455%/	-+646//8	5.79026
. 4	-4 03340 -4 07077	787262	3+6662
• <del>•</del>	-7 00000	-1.3289	3+34143
• TU .5	-/+V00V2 7 71+^7	-1+00044	3.42158
•J 、55	-7 EAA77	-1+76401 	3.34657
. 4	-/+J9V/2 7 77715	-2 -20/44	3.34703
.45	-/+///13	-2+27044 -2 2004	0+48071 E 77745
.7	-0+V1703 -0-27701	TZ+ZÖZ4 …0 48500	0./3/45
・/ 、フロ	-0+2/071 -0 6/750	-1 05007 -1 05005	0+11802
•••	-0+04002 -0:07570	-1 744A4	0+00046
•0	-0+03J/7 -0.14718	TI+30340 - 476/40	/ 4/433
	- <b>147037</b> 3	-, 0JJ042	0.02/01

T-STAR	= 1			
N-STAR		S-STAR	H-STAR	G-STAR
• 05		-4.69871	1,19286	5.89157
+1		-5.25423	•872078	6.12631
.15		-5.61861	• 480824	6.09944
•2		-5.9076	.142519	6.05012
•25		-6,15732	180032	5.97728
•3		-6.38525	497457	5.8878
•35		-6.60368	81385	5.78983
• 4		-6.81855	-1.12576	5.69278
•45		-7.03623	-1.43361	5.60262
•5		-7.25929	-1.70269	5.55661
•55		-7,48893	-1.90343	5.58551
•6		-7.72537	-1.98762	5.73775
• 65		-7,96808	-1.95686	6.01121
•7		-8.22214	-1.81499	6.40715
•75		-8.49176	-1.5052	6.98656
•8		-8.78401	997083	7.78693
•85		-9.11139	255567	8.85582
T-STAR	= 1.05			
N-STAR		S-STAR	H-STAR	G-STAR
•05		-4.6495	1.21768	5.86738
•1		-5.20504	•919899	6.12494
.15		-5.56941	.55081	6.12022
•2		-5.85841	.234201	6.09261
.25		-6.10812	671742E-01	6.04095
•3		-6.33606	362424	5.97364
•35		-6.55447	6552	5.89927
.4		-6.76934	942021	5.82732
.45		-6.98703	-1,223	5.76403
•5		-7.2101	-1.46586	5.74424
.55		-7.43975	-1.6427	5.79705
•6		-7.67618	-1.70828	5,9679
.65		-7.91888	-1.66237	6.2565
•7		-8.17294	-1.50661	6.66633
.75		-8.44257	-1.18601	7,25657
•8		-8.73484	667455	8.06738
.85		-9.06222	.08829	9,15051
· ·				/120002
T-STAR	= 1.1			
N-STAR		S-STAR	H-STAR	G-STAR
•05		-4.60264	1.24057	5.84321
•1		-5.15819	•963321	6.12151
.15		-5.52256	<u>•614371</u>	6.13694
.2		-5.81155	.317501	4.12905
•25		-6.06127	-353809F-01	6.09665
.3		-6.28921	239718	6.04949
.35		-6.50762	511029	5.99459
•4		-6.72249	775043	5.94745
.45		-6.94019	-1.03161	5.90857
•5		-7.16325	-1.2506	5.91244
•55		-7.3929	-1.40571	5,98719
•6		-7.62934	-1.45470	6.17AOA
.65		-7.87203	-1, XQA707	6. A7771
.7		-8,1261	-1.22432	A, 99979
.75		-8,30577		7 80004
.8		-8,292	-+070004 	7 + 47700 0 2001 A
.85		-9,01574	-+30/03J . Annoaq	0+32014
			+ 777077	7 4 7 LOZI

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T-STAR =	1.15		
N-STAR	S-STAR	H-STAR	G-STAR
•05	-4.55792	1.26122	5.81915
• 1	-5.11345	1,00293	6.11639
•15	-5.47783	•672372	6.1502
•2	-5,76683	•393509	6.16034
•25	-6.01654	<b>•128971</b>	6.14551
•3	-6.24449	127726	6.11676
•35	-6+4629	379452	6.08345
•4	~6,67778	-+622639	6.05514
• 45	-6.89546	-•856901	6.03856
•5	-7.11852	-1.05412	6.0644
•55	-7.34818	-1.18938	6.1588
•6	-7,58461	-1.22261	6,362
•65	-7.82732	~1.15039	6.67693
•7	-8.08139	970453	7,11093
+/5	-8.351	631007	7.71999
•8	-8,64328	094336	8.54894
•85	-8,97065	•686153	9.6568
T-STAR =	1.2		
N-STAR	S-STAR	H-STAR	G-STAP
•05	-4.51512	1.28014	5.79524
•1	-5.07066	1.03921	6.10987
•15	-5,43504	•725504	6.16055
•2	-5.72402	•463173	6.18719
<b>•25</b>	-5.97374	•214736	6.18848
+3	-6.20169	250809E-01	6.1766
• 35	-6.42011	-+25885	6,16126
•4	-6.63499	-+482959	6.15203
+45	-6.85267	-+696783	6.15589
•5	-7.07573	874035	6.2017
+55	-7,30539	991103	6.31428
•6	-7.54183	-1.01018	6.53164
+65	-7.78454	926448	6.85809
•7	-8.0386	735934	7.30266
+75	-8.30822	388258	7.91997
•8	-8,6005	·156338	8.75684
•85	-8,92785	•947669	9.87552
T-67A8 -	1 96		
N-CTAD	I+2J C_CTAD	11 OTAG	
.05	- A A7400	H-51AK	G-SIAR
•••		1.427/03	5 + / / 161
• •	-5 70A	1.07208	6+1022
• • • •	-5.40790	•//4382	6+16838
• <u>~</u> .25	-5.07071	• 32/ 229	6+21022
.7	-4 14045	• 273927	6+22634
・J 、ズ5	-4 77000		6+22998
• 30 . A	-4 59704	~+14/916	6.23116
* 7		-+304443	6.2395
• <del>•</del> • •		-+349482	6.26216
.55	-7+V34/1 -7.94/1	-•/V8382 000407	0.32633
	/+2043J _7.5000		0.40060
.45	-7.7A7A0	_+014/37 ~.790////	0+006V4
.7	-7,99754	~+/2V4V4 ~.500170	7 47770
.75	-8.94710	+UZVI/Z 128075	7 + 77/37
•8	-8.55944		Q.QAZA4
.85	-8.88683	1.18822	10.075
•	2.00000	LILUULL	· ·

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T-STAR =	1.3		
N-STAR	S-STAR	H-STAR	G-STAR
•05	-4+43469	1.31355	5.74824
•1	-4,99023	1.10334	6.09357
•15	-5.35461	<b>.</b> 819463	6.17407
•2	-5.64361	•586323	6.22993
•25	-5.89332	.366412	6.25973
•3	-6.12126	•156446	6.27771
•35	-6.33969	04555	6.29414
•4	-6.55455	235867	6.31869
• 45	-6,77225	413542	6.35871
•5	-6,99532	555489	6.43983
•55	-7+22497	640365	6.5846
•6	-7+4614	634397	6.82701
•65	-7.7041	530274	7,17383
+7	-7.95817	321049	7.63712
•75	-8.2278	•411975E-01	8,26899
•8	-8.52007	•579824	9.11989
•85	-8.84746	1.41031	10.2578
T-STAR =	1.35		
N-STAR	S-STAR	H-STAR	G-STAR
•05	-4,39681	1.32836	5.72516
, <b>•1</b>	-4.95234	1.13181	6.08415
•15	-5.31673	<b>.</b> 861176	6.17791
•2	-5.60571	.641039	6.24675
•25	-5.85544	<b>•433788</b>	6.28922
•3	-6.08338	•237089	6.32047
•35	-6.3018	.492261E-01	6.35102
•4	-6.51668	126097	6.39058
• 45	-6.73437	28769	6.44668
•5	-6.95744	-+413949	6.54349
•55	-7,18709	484518	6.70257
•6	-7.42353	467421	6.95611
•65	-7.66623	354245	7.31199
•7	-7.9203	136707	7.78359
•75	-8.18992	.232019	8.42194
•8	-8,48219	•796891	9.27908
•85	-8.80956	1,61587	10.4254
T-STAR =	1.4		
N-STAR	S-STAR	H-STAR	G-STAR
•05	-4.36029	1.34212	5.70241
•1	-4.91584	1.15823	6.07407
.15	-5.28021	+B99936	6.18014
•2	-5.56922	.691823	6.26104
•25	-5.81893	•496352	6.31528
•3	-6.04688	•311966	6.35884
<b>،3</b> 5	-6.26529	•137223	6.40251
•4	-6.48017	241531E-01	6.45601
• 45	-6•69786	170825	6.52703
•2	-6.92092	282499	6.63842
•55	-7.15058	339797	6.81078
+6	-7.38702	312365	7.07466
•65	-7.62971	190772	7.43894
•7	-7.88378	•03449	7,91827
•75	-8.15341	•409226	8.56264
•8	-8.44568	<b>•979876</b>	9,42555
•85	-8.77305	1.80678	10.5798

T-STAR :	= 1.45			
N-STAR		S-STAR	H-STAR	G-STAR
•05		-4.3251	1.35489	5.67999
•1		-4.88064	1.18282	6.06345
•15		-5.24501	•935971	6.18098
•2		-5.53401	•739102	6.27312
•25		-5.78372	•554581	6.3383
•3		-6.01167	•381671	6.39334
•35		-6.23009	•219124	6.44922
• 4		-6.44496	<b>₊707327E-01</b>	6.51569
•45		-6.66266	620529E-01	6.60061
•5		-6.88572	160154	6.72557
•55		-7.11537	205078	6.9103
•6		-7,35181	168018	7.18379
+65		-7.59451	-,385966E-01	7,55591
•7		-7.84858	•193843	8.04243
•75		~8,11821	•57418	8.69239
•8		-8.41049	1.15021	9.5607
•85		-8.73785	1.98449	10,7223
T-STAR :	= 1.5			
N-STAR		S-STAP	H-STAD	C_CTAD
.05		-4.2911	1.36681	5 45701
.1		-4.84443	1,20577	4.05270
.15		-5.21103	.949594	4 10047
.2		-5.5	.783225	6.39737
.25		-5.74972	. 408922	4.75044
•3		-5.97768	.446699	6.47479
.35		-6.1961	.295557	A. 40145
• 4		-6.41098	.159248	A.57025
.45		-6.62867	.394531E-01	A. 44812
•5		-6.85173	045979	A.80575
•55		-7.08138	- 7975745-01	7 00303
.6		-7.31782	- 77705765-01	7 9045
• 65		-7.56053	.103402	7.204J 7.22707
•7		-7.81459	.342556	8.15715
•75		-8.08422	.728127	8.81274
•8		-8.37649	1,3092	0.48540
•85		-8.70387	2.15029	10.8542
T-STAR =	= 1.55	C.CTAD	11 6745	0.0745
05		3-31AK	H-SIAK	G-STAR
.1		-4+23821	1+3//9/	5.63618
15		-4+813/3	1.22/22	6.04096
*13		-3+1/813	1.00107	6.1/92
.25		-3+40/12	• 824473 / FD7 47	6+27161
*25			•037/43	6.3/659
(J 75		-2+744/7	+30/333	6.45234
.4		-4 77000	+30/03/	6+53027
. 45		-0.3/8V7	+ 2421VD	6+6202
•7J .5		-0+J7J/0 _4 01005	+134433	6.73021
.55		-7.01000	• 0V0324E-V1 7024405 A4	0+0/768
		-7.7047	+302010E-V1 .074047E-A4	7.000/6
.45		-7+20473	•720002ETVI .774740	7+3//03
•7		-7,78171	+ ∠∂0240 , <u>A</u> 01 ∠70	/+/037 9.94770
.75		-8.05177	+ 7010/0	0+20337
48		-8.74741	1 A5703	0.001E7
.85		-8.47000	2 + 73/72 2 - 305A7	7+07133
			4+VVU7/	****7/0J

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T-STAR =	1.6		
N-STAR	S-STAR	H-STAR	G-STAR
•05	-4.22638	1.38841	5.61479
•1	-4.78191	1.24733	6.02924
•15	-5.14631	1.03055	6.17686
•2	-5.43529	•863166	6.29845
•25	-5+68501	+707396	6.3924
•3	-5.91295	+564587	6.47754
•35	-6.13137	•434104	6.56547
• 4	-6.34626	•319761	6.66602
•45	-6.56394	•223464	6.7874
•5	-6.78701	•160972	6.94798
•55	-7+01667	+14851	7,16518
•6	-7+2531	•210833	7.46393
•65	-/+4958	+360804	7.85661
•/	-/•/4988	.612112	8,36199
•/5	-8.0195	1.00715	9,02665
•8	-8,31178	1.59735	9,90912
.85	-8.63914	2+45091	11.0901
T-STAR =	1.65		
N-STAR	S-STAR	H-STAR	G-STAR
•05	-4.19554	1.39822	5,59375
•1	-4.75109	1.26619	6.01728
.15	-5.11546	1.05825	6,17371
.2	-5.40447	.899444	4.30393
.25	-5.45418	.750130	4.40473
.3	-5,88213	. 419137	4.50027
.35	-6.10054	. 497041	6.59758
.4	-6.31542	.392696	6.70811
.45	-6.53311	.307069	6.84018
۰.c	-6.75617	.255023	7.01119
.55	-6,98582	.25208	7.2370
•6	-7.22227	.321782	7.54405
.65	-7.46496	.477789	7.94275
.7	-7.71903	.734427	8.45366
.75	-7.98866	1,13307	9.12243
.8	-8,28094	1.72831	10.0093
.85	-8.40831	2.58752	11,1958
100	0100001		11+1/50
T-STAR =	1.7		
N-STAR	S-STAR	H-STAR	G-STAR
•05	-4.16562	1.40744	5,57306
•1	-4,72116	1.28396	6.00513
•15	-5.08554	1.08431	6,16985
•2	-5.37454	•933658	6.3082
•25	-5.62425	•794251	6.4185
•3	-5.8522	•668563	6.52076
•35	-6.07062	•556291	6.62692
•4	-6.2855	•461337	6.74683
•45	-6.50318	•385771	<b>6.88</b> 896
•5	-6,72626	•343529	7.06979
•55	-6.9559	•349551	7,30545
•6	-7.19235	•426217	7.61856
•65	-7.43505	•587877	8,02293
•7	-7.68911	849935	8.53904
•75	-7,95874	1.25332	9,21207
•8	-8.25101	1.85158	10.1026
•85	-8.57839	2.71611	11.2945
•			•

T-STAR	= 1.75			
N-STAR		S-STAR	H-STAR	G-STAR
.05		-4.13658	1.41613	5.55271
•1		-4.6921	1.30072	5,99283
.15		-5.05649	1.10888	6.16537
•2		-5.34548	•965902	6.31138
•25		-5.59519	•833961	6.42916
•3		-5.82315	•716092	6.53924
•35		-6.04158	•612149	6.65373
•4		-6.25644	•526062	6.7825
•45		-6.47414	•459961	6.93411
•5		-6.69721	• 426993	7.1242
•55		-6.92687	•441431	7.3683
•0		-/+1633	•52468	7.68798
• 65		-7,40601	•69168	8.09769
•7		-7+66007	•958631	8.6187
•/5		-/+72707	1.36585	9+29555
• 8 0 E		~8+22196	1.96779	10.1897
-80		-8.34735	2.83737	11,3867
T-STAR	= 1.8			
N-STAR		S-STAR	H-STAR	G-STAR
•05		-4.10835	1.42434	5.53269
•1		-4,6639	1.31651	5.98041
•15		-5.02828	1.13206	6.16034
•2		-5.31728	•996312	6.31359
•25		-5.567	.871425	6.43842
• 3		-5.79493	•760973	6.5559
•35		-6.01336	•664893	6.67826
•4		-6+22824	•587154	6.8154
•45		-6.44593	.530021	6,97595
+5		-6+66899	•505801	7.17479
• 55		~6.87864	•52822	7.42686
+0		-/.13309	+61/653	7.75274
•00		-/+3///9	•/89/11	8.16/5
*/		-7+03180	1.00129	8.67313
•/5			1+4/21	7:3/307
+0		-0+173/0		10+2/13
+QJ		-0,J2114	2+75182	11+4/3
T-STAR	= 1.85			
N-STAR		S-STAR	H-STAR	G-STAR
•05		-4.0809	1.4321	5.513
•1		-4.63645	1.33147	5,96792
•15		~5.00082	1.15401	6.15483
•2		-5.28983	1.0251	6.31493
•25		-5.53955	•906891	6.44644
•3		-5,76748	•803425	6.57091
•35		-5.9859	•714806	6.70071
+4		-6.20079	•644968	6.84575
•40		-6.41846	•596319	7.01478
•0		-0+04100	• 38036	7+22189
• 00 . A		-7.107110	+010317	/+4810
•0		-7.35074	+/VJ022	7+81325
.7		-7.4044	+002942 1.18049	0+232/0 0 72904
.75		-7,87477	1 + 1J042 1 . 5794 <i>A</i>	0, 44440
.8		-8.1447	1+J/204 9,19177	7 + 7 7000 1 Å , 7 474
.85		-8.49348	3.04014	11.5570
		~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	<b>444410</b>	

T-STAR =	1.9		
N-STAR	S-STAR	H-STAR	G-STAR
•05	-4.05421	1.43943	5.49364
• 1	-4.60973	1.34564	5.95537
•15	-4.97412	1,17478	6.1489
+2	-5,26311	1.05237	6.31548
•25	-5.51283	•940489	6.45332
•3	-5.74078	•843628	6.58441
•35	-5.95919	•762075	6.72126
+4 AE	-6.1/408	•699723	6.8738
+40 E	-6.41483	•657084	7.05086
*J .55	-0·01402 	+030783	7 57054
. 6	-7.09097	+0000/3	7+JJZJO 7 04004
.45	-7.33344	+/007JJ 07/075	7 + 00700
•03	-7.5777	1.2504	0+27371
.75	-7.84732	1.44788	0.5152
•PO	-8,13959	2.27947	10.4193
.85	-8,46696	3.14973	11.4297
100	01-10070	0.10270	
T-STAR =	1.95		
N-STAR	S-STAR	H-STAR	G-STAR
.05	-4.02818	1.4464	5.47458
•1	-4.58372	1.35907	5.94279
•15	-4.94811	1.19449	6.1426
•2	-5.23711	1.07822	6.31533
•25	-5.48682	•972352	6.45917
+3	-5.71477	•881773	6.59655
•35	-5.93319	•806901	6.74009
•4	-6.14805	•751695	6+89974
•45	-6+365/5	•718656	7.08441
+0 55	-0.36683	•/1/962	/+306/9
+33		•/61849	7.58032
•0	-7.00471	+86/773	7.9227
•00	-7.6517	1+00000	8+33124
.75	-/+001/	1+33/00	8.88733
.8	-9.11759	10/30/2 7 77707	7+3/733
.85	-9.11335	2.03/27/	11 701
100	0+44770	3+20007	11+/01
T-STAR =	2		
N-STAR	S-STAR	H-STAR	G-STAR
•05	-4.00282	1.45302	5.45585
•1	-4.55837	1.37183	5.9302
.15	~4.92275	1.21323	6.13598
•2	-5.21174	1.1028	6.31454
. •25	-5.46147	1.00262	6+46409
•3	-5.68941	•918024	6.60744
•35	-5.90783	•B49499	6.75733
• 4	-6.12271	•801026	6.92374
• 45	-6.3404	•775238	7,11564
•5	~6+56347	•78161	7.34508
100	~6.79312	•831936	7.62505
+0	-/+02956	•943074	7.97264
+00	-/.2/225	1.1328	8.40505
• /	-/.32033	1.42059	8,94692
•/5	-/./9596	1.84404	7.64
+ 0	-8+V8822	2+46161	10.5498
+60	~8+41201	3.35233	11,/681

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T-STAR =	2.05		
N-STAR	S-STAR	H-STAR	G-STAR
•05	-3.97812	1.45929	5.43741
•1	-4.53364	1.38397	5.91761
•15	-4.89802	1.23104	6.12906
•2	-5.18701	1.12617	6.31319
•25	-5.43673	1.03142	6.46815
• <u>)</u>	-5.66467	•952507	6.61718
+33	-3+8831	•890022	6.77312
• 4		•84/965	6.94596
• • • •	-4 57074		7,144/3
.55	-6+33878	+042141	7+3809
•6	-7.00483	1.01451	8.01934
• 65	-7.24756	1.20808	R.45547
•7	-7.50162	1.49944	9,00106
•75	-7.77125	1.92566	9.69691
•8	-8.06352	2.54589	10.6094
•85	-8,39089	3.44047	11.8314
1-STAR =	2.1		
-05	5-51AK -7 85705	M-51AR	G-STAR
.1		1+46032	5.4192/
•± .15		1+37334	2.70204
.2	-5,14289	1.14940	0+12187 2 71171
.25	-5.41263	1.05881	4.47145
•3	-5.64058	.9853	6.62588
•35	-5.85876	•928616	6.78758
+4	-6.07383	•892704	6.96653
• 45	-6.29155	•880309	7.17186
•5	-6.51462	<b>•899804</b>	7.41443
• 55	-6,74427	•96208	7.70635
•6	-6.98072	1.08251	8,06324
•65	-7.22341	1.27981	8,50322
•7	-7.47747	1.57456	9.05203
•75	-7.74711	2.00342	9.75053
+8	-8.03935	2.62621	10.6656
•80	-8+366/7	3,52423	11.891
T-STAR =	2,15		
N-STAR	S-STAR	H-STAR	G-STAR `
•05	-3,93045	1.47098	5.40143
•1	-4,48597	1.40652	5.8925
•15	-4.85036	1.26414	6.1145
•2	-5,13933	1.16963	6.30897
•25	-5.389	1.08503	6.47403
•3	-5,61693	1.0167	6.63362
•35	-5.83542	•965393	<b>6.8</b> 0081
• 4	6.05028	•935316	<b>6 • 78</b> 56
• 45	-6.26798	•929201	<b>7.1</b> 9718
• 3	-6.49109	•95475	7.44584
+ 2 3 . 4	-6,72069	1.02263	7.74333
*0	-0+7J/16 -7.10004	1.14/37	8.10454
.7	-7.417701 -7.45705	1+34824 1 2824 A	8+34804
.75	-7.70754	▲ + 09014 ウ. ハツッミメ	7+10009
•8	-8.01589	2+V//34 2,76949	7+0V11 10,7104
•85	-8.34315	3,40412	11.9473
A .		wywy i da fa	******* <b>U</b>

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