A THEORETICAL INVESTIGATION OF THE EFFECT OF INTERMOLECULAR CORRELATIONS UPON PROPERTIES OF SIMPLE LIQUIDS FROM X-RAY DIFFRACTION

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TRUE SCIENCE TEACHES, ABOVE ALL, TO DOUBT, AND TO BE IGNORANT.

Miguel de Unamuno

"The Tragic Sense of Life"

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To put down the words that belong on this page is the most difficult task of all. For, how is one to express gratitude in a few short sentences?

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ABSTRACT

This work reports a theoretical study on the effect of including intermolecular correlations in x-ray scattering data from simple liquids.

An instantaneous configuration-dependent scattering factor is defined for a molecule in a liquid. Using statistical mechanics and physical principles, an expression is derived that corrects the usual scattering equations, for both coherent and incoherent radiation.

Computations, using the new result, were done on liquid helium and argon. Comparison of correlated scattering factors and isolated molecule scattering factors show significant deviations, especially for larger angles of scattering. Incorporating correlation effects into scattering data for these liquids, the resultant radial distribution function peak is depressed an average of 1% and the potential energy is lowered by 5%. Treatment of data in this manner leads to better agreement with theoretical predictions.

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Chapter I - Theory of X-Ray Scattering from Uncorrelated Molecular Liquids

A. Introduction

Modern theories of the properties of matter rely upon the study of atoms and molecules. From their individual properties and knowledge of the forces which they exert on each other, it is possible to calculate how matter in bulk behaves. The inherent difficulty is to find some way of calculating the effects of the interactions, between the enormous number of molecules, in any quantity of matter on which it is suitable to experiment. Statistical mechanics bypasses this difficulty by considering all possible states in which a system can be found and by finding the probability for the realization of each state. In order to make practical calculations on the basis of theoretical developments, it is further necessary to assume an analytic form for the interaction potential. (Discussions of the various empirical potentials in use may be found in Hirschfelder, Curtiss and Bird[1], Margenau and Kestner[2], and Hirschfelder[3].)

Having performed these computations, it remains the task of the experimentalists to verify their accuracy. Relating the properties of matter to structure relies greatly on the various experimental methods of "seeing" atoms. One of these, diffraction, has provided most of what is now known of atom sizes and arrangements in the solid and gaseous states.

It was recognized as early as 1923 by Keesom and de Smedt[8], that x-ray diffraction techniques could be a source of quantitative information of the molecular structure of liquids. The analyses required for the interpretation of the diffraction patterns were developed by Debye[9], Zernike and Prins[10], and Menke[11]. X-ray diffraction measurements have been made on quite a number of liquids, liquid solutions, and liquid metals (e.g., Schmidt and Tompson[4], Gingrich[5], Furukawa[6], and Pings[7].)

Unlike the crystalline state, in liquids there is no long-range molecular or atomic order, and the molecular positions must be described by probabilities instead of fixed distances as in crystal structure. Thus, the experimental x-ray scattering data from a liquid is used to compute a function $g(R)$, known as the pair correlation function or the radial distribution function (RDF), which is regarded as a measure of the average probability that molecules in the liquid will be separated by a distance R.

The radial distribution function and other properties obtained from experiments using these analyses appear to be reasonable when compared with theoretical predictions (Chen[12] and Ree[13]). However, discrepancies do occur, especially in the appearance of spurious peaks in the radial distribution function and variation of the potential well depths (Rowlinson, et al.[54]). An explanation of how these effects may arise due to mistreatment of data has been given by Kirstein[14]. As more experimental data became available, it was realized that the usual assumption of spherical charge distributions for the scatterers, especially in the case of complex molecules, might produce significant deviations between the true and predicted intensities. McWeeny[15-18] studied the variation in the scattered amplitude from free and bound atoms. Freeman[19] compared amplitudes of spherical and nonspherical charge distributions. Wilkinson and Brown[20] showed how scattering amplitudes in a structure may be evaluated as functions of the scattering vector $\bar{s}$. Dawson[21] studied the deviation of the scattered amplitude between prepared hybrid valence states and the ground state results.

Recently, Steele and Pecora[22] have deduced an expression for the scattering cross section of a liquid consisting of nonspherical molecules. Blum and Torruela[23] have extended this expression into a form which is independent of any particular reference frame used to define the orientation of the molecules. Calculations for the effects of molecular orientation, based upon the work of Steele and Pecora, have been performed by Morrison and Pings[24].

There is an additional effect to be considered. The molecules are continuously moving with respect to each other due to thermal energy. The magnitude of these motions may be quite large. However, unlike dilute gases, the intermolecular separations may now be small enough to cause the charge distribution of any given molecule to be correlated with the instantaneous configuration of its neighbors and of the system. Depending upon the presence of permanent or induced dipoles, or both, the distribution of charge, especially in the outer and valence shells, may become distorted. Cromer[25], using different atomic models, has shown that the scattering amplitude is sensitive to this behavior.

The present work extends the above analyses of x-ray scattering from a liquid. Using configuration dependent molecular charge distributions, and by applying physical and statistical principles, an expression is obtained for the coherent scattering intensity which includes this effect. It is also shown how the incoherent intensity should be treated. Then, x-ray scattering data for liquid helium and liquid argon are analyzed in light of the new results.

The usual theory of x-ray scattering will be presented in the remainder of this chapter. Readers familiar with these results may proceed to the next chapter without loss of continuity. Chapter II shows how the usual theory of x-ray scattering for liquids may be extended to take account of intermolecular correlations. The results, with application to helium and argon, are discussed in Chapter III. Conclusions and recommendations are in Chapter IV.

B. The Single-Electron Atom

If a beam of radiation falls on a target and wavelets scattered by different atoms have similar amplitudes and phases, then the scattered waves will interfere and the target will act as a diffraction grating.

Almost any kind of radiation may be used: electrons, neutrons, or electromagnetic waves (x-rays, light).

An electron beam scatters from the nuclear and electronic charge distributions. Neutrons scatter from the target nuclei. X-rays and light both interact with the nuclear and electronic charges, the contribution of the former being usually neglected since the amplitudes are in inverse ratio to the masses.

The quantum mechanical calculation of the coherent and incoherent radiation from electrons, under the influence of an electromagnetic wave, was first carried out by Wenzel[26] and Waller[27]. An outline of the solution follows.

The incident radiation is assumed to consist of a monochromatic plane polarized wave, traveling in the direction of the unit vector $\bar{u}$. The electric intensity is given by the real part of

$$\bar{E} = \bar{E}_o \, e^{i(\omega t - \bar{s}\cdot\bar{r})} \tag{1}$$

where $\omega = 2\pi f$, f being the frequency of the incident radiation; $s_o = \omega\bar{u}/c$; c is the speed of light; $\bar{r}$ is the vector distance from some point in the scatterer, e.g., the nucleus if the wave is scattered by an atom.

The electric intensity $\bar{E}$ is connected with the vector potential $\bar{A}$ and scalar potential ϕ by

$$\bar{E} = -\frac{1}{c}\frac{d\bar{A}}{dt} - \bar{\nabla}\phi \tag{2}$$

For an electron of mass m and charge e in these fields, the appropriate form of the non-relativistic Hamiltonian is

$$H = \frac{-\hbar^2}{2m}\nabla^2 - \frac{\hbar e}{imc}\bar{A}\cdot\bar{\nabla} + \frac{e^2}{2mc^2}\bar{A}\cdot\bar{A} + e\phi \tag{3}$$

where h is Planck's constant and $\hbar = h/2\pi$.

The wave field is to be treated as a small perturbation, so that terms involving the square of the vector potential may be neglected. The scalar potential of the wave field is zero.

The Hamiltonian is split into unperturbed and perturbation operators. The unperturbed operator is

$$H_I = \frac{-\hbar^2}{2m} \nabla^2 + V(r) \tag{4}$$

V(r) being the potential energy of the particle.

The perturbation operator is

$$H_{II} = \frac{-\hbar e}{imc} \overline{A} \cdot \overline{\nabla} \tag{5}$$

The solution of the Schrodinger wave equation

$$H_I\psi = i\hbar \frac{\partial\psi}{\partial t} \tag{6}$$

for the unperturbed operator yields various solutions $\psi_1 e^{-i\varepsilon_1 t/\hbar}$, $\psi_2 e^{-i\varepsilon_2 t/\hbar}$, $\cdots$, $\psi_n e^{-i\varepsilon_n t/\hbar}$ corresponding to the different stationary states of energies $\varepsilon_1, \varepsilon_2, \cdots, \varepsilon_n$.

For a system that is perturbed, the solutions to the wave equation

$$H_I\Phi + H_{II}\Phi = i\hbar \frac{\partial\Phi}{\partial t} \tag{7}$$

are sought.

Whatever the solution Φ may be, it can always be expressed as a linear combination of wavefunctions satisfying the unperturbed equation (6). Thus,

$$\Phi = \sum_m a_m \psi_m e^{-i\varepsilon_m t/\hbar}$$

where $|a_m|^2$ is the probability that as a result of the perturbation the atom is in the state m .

To determine the coefficients a_m , substitute (8) in (7) and, making use of (6), obtain

$$\sum_m a_m H_{II} \psi_m = i\hbar \sum_m \psi_m \frac{\partial a_m}{\partial t} \tag{9}$$

Assuming the wavefunctions to be orthogonal and normalized, multiplying both sides of (9) by ψ_k^* and integrating over all space[†], the exact result

$$i\hbar \frac{\partial a_k}{\partial t} = \sum_m a_m \int \psi_k^* H_{II} \psi_m \, dv \tag{10}$$

is obtained.

If an atom were in the state n, $a_n = 1$ and all the other coefficients would be zero. The right hand side of (10) contains all the coefficients a. As a first approximation, a_n is taken as 1 and all the other coefficients are assumed negligible, resulting in

$$\begin{aligned} i\hbar \frac{\partial a_k}{\partial t} &= \int \psi_k^* H_{II} \psi_n \, dv = \\ &= e^{i(\varepsilon_k - \varepsilon_n)t/\hbar} H_{nk} \end{aligned} \tag{11}$$

where

$$H_{nk} = \int \psi_k^* H_{II} \psi_n \, dv \tag{12}$$

The calculation of H_{nk} requires an expression for the vector potential. By (2), since $\phi = 0$,

$$\bar{A} = -\frac{c\bar{E}_o}{2\omega i} e^{i(\omega t - \bar{s}_o \cdot \bar{r})} + \frac{c\bar{E}_o}{2\omega i} e^{-i(\omega t - \bar{s}_o \cdot \bar{r})} \tag{13}$$

[†] Unless otherwise indicated, it will be implicitly understood that all integrals are to be taken over configuration spaces.

Denote the component of the gradient in the direction of the electric field vector by x_o , the direction of x_o being perpendicular to $\overline{u}$. Then H_{nk} may be written

$$H_{nk} = -\frac{\hbar e}{2m\omega} |\overline{E}_o| \{B_{nk} e^{i\omega t} + B^*_{kn} e^{-i\omega t}\} \tag{14}$$

where

$$B_{nk} = \int \psi^*_k e^{-i\overline{s}_o \cdot \overline{r}} \frac{\partial \psi_n}{\partial x_o} dv \tag{15}$$

Using (14), the integration indicated by (10) may be carried out on the assumption that $a_n = 1$, to give the result

$$\Phi = \psi_n e^{i\varepsilon_n t/\hbar} + \frac{e|\overline{E}_o|}{2m\omega} \sum_{k\neq n} \left\{ \frac{B_{nk} e^{i(\hbar\omega-\varepsilon_n)t/\hbar}}{\omega_{kn} + \omega} + \frac{B^*_{kn} e^{-i(\hbar\omega+\varepsilon_n)t/\hbar}}{\omega_{kn} - \omega} \right\} \tag{16}$$

where $\omega_{kn} = (\varepsilon_k - \varepsilon_n)/\hbar$ is the circular frequency corresponding to the transition of the atom from the state k to the state n .

The radiation scattered by the atom is calculated from the laws of classical electrodynamics.

Let $\dot{\overline{J}}$ be the oscillatory current density, of circular frequency ω , at a point Q , specified by the vector $\overline{r}$ from the origin O . The field at a point P , distant R from O is required. R is large in comparison with the dimensions of the region about O within which the current density is appreciable.

$\overline{s}_1 = \omega_1 \overline{u}_1/c$ where ω_1 is the circular frequency of the scattered radiation in the direction of the unit vector $\overline{u}_1$. Then, the result from classical electrodynamics is that the amplitude of the scattered radiation field E_s, at P, may be derived from an electric moment at O by

$$E_s = \frac{\omega^2}{c^2} M \tag{17}$$

where

$$M = \pm \frac{1}{i\omega} \int J_p \, e^{i\bar{s}_1 \cdot \bar{r}} \, dv \tag{18}$$

and J_p is the component of $\bar{J}$ perpendicular to $\bar{s}_1$ and contains the time through the factor $e^{\pm i\omega t}$. The exponential term in the integrand of (17) allows for the effect on the phase of the scattered wave of the varying distance of the element of volume dv from O.

Equations (4) and (5) are placed in (7) and the result multiplied by Φ^*. The conjugate equation for Φ^* is multiplied by Φ. If the one is subtracted from the other, the result is

$$\frac{\hbar^2}{2m} (\Phi\nabla^2\Phi^* - \Phi^*\nabla^2\Phi) + \frac{i\hbar e}{mc} \bar{A}\cdot(\Phi^*\nabla\Phi + \Phi\nabla\Phi^*) = i\hbar \frac{\partial}{\partial t} (\Phi\Phi^*) \tag{19}$$

For a plane electromagnetic wave, div $\bar{A} = 0$. The above result may then be written,

$$\text{div} \left\{\frac{i\hbar e}{2m} (\Phi\nabla\Phi^* - \Phi^*\nabla\Phi) - \frac{e^2}{mc} \bar{A}\, \Phi\Phi^*\right\} + \frac{\partial}{\partial t} (e\Phi\Phi^*) = 0 \tag{20}$$

Comparing (19) with the equation of continuity, the Schrodinger current density is seen to be given by

$$\bar{J} = \frac{i\hbar e}{2m} \{\Phi\nabla\Phi^* - \Phi^*\nabla\Phi\} - \frac{e^2}{mc} \bar{A}\Phi\Phi^* \tag{21}$$

1. Coherent Scattering

If the frequency of the incident radiation ω is large in comparison with any of the atomic transition frequencies ω_{kn}, the terms under the summation sign in (16) are then small. Moreover, they appear in the expression for the current density in terms of order E_o^2, which is itself a small quantity since the field is to be considered as a small perturbation.

The first term in (21) contributes nothing to the scattering since it does not contain the time. The current density is then reduced to $-(e^2/mc)|\psi_n^2|\overline{A}$ if the atom is in the state n.

Making use of (13), it is readily seen that the current density vector is proportional to and in the direction of the incident electric field vector $\overline{E}$. Substituting the value of the current in (18),yields the scattering amplitude

$$Y_{coh} = \frac{-e^2}{mc^2} \frac{E_{op}}{R} e^{i\omega t} \int |\psi_n|^2 e^{i\overline{s}\cdot\overline{r}} dv \tag{22}$$

where $\overline{s} = \overline{s}_1 - \overline{s}_o$, and E_{op} is the component of $\overline{E}_o$ perpendicular to $\overline{s}_1$. $E_{op} = |\overline{E}_o|$ if $\overline{E}$ is perpendicular to the plane containing both $\overline{s}_o$ and $\overline{s}_1$. $E_{op} = |\overline{E}_o|\cos(\theta)$, when $\overline{E}$ is in the plane containing $\overline{s}_o$ and $\overline{s}_1$. θ is the angle between the incident and scattered directions.

The intensity of coherent scattering of unpolarized radiation, by an atom in the state n is

$$I_{n,n}(s) = Y_{coh} \cdot Y^*_{coh} = \frac{|\overline{E}_o|^2}{R^2} \left(\frac{e^2}{mc^2}\right)^2 \left(\frac{1+\cos^2\theta}{2}\right) |f_{n,n}(s)|^2 \tag{23}$$

where

$$f_{n,n}(s) = \int |\psi_n|^2 \, e^{i\bar{s}\cdot\bar{r}} \, dv \tag{24}$$

The quantity $f_{n,n}(s)$ is called the scattering factor for the electron in the state n .

The term multiplying the scattering factor is the intensity scattered by a classical electron under the same conditions (Thomson[28]).

The intensity of coherent scattering relative to that of a classical free electron is given by

$$I_{coh}(s) = |f_{n,n}(s)|^2 \tag{25}$$

2. Incoherent Scattering

Incoherent scattering is associated with processes in which the electron undergoes a transition from the initial state n to other final states m . The incident frequency is subject to the same restrictions as the coherent scattering.

The current density associated with a transition from state n to m under the influence of the perturbing field is

$$\bar{J}_{n,m} = \frac{i\hbar e}{2m}(\Phi_n \bar{\nabla}\Phi_m^* - \Phi_m \bar{\nabla}\Phi_n^*) - \frac{e^2}{mc}\,\bar{A}\;\Phi_n\Phi_m^* \tag{26}$$

The first term in the equation above is dependent upon the time and is associated with the spontaneous emission from the atom. The effect of the perturbation is contained in the second term. Using methods analogous to those discussed above, the intensity, relative to that from a classical electron scattering under the same conditions, associated with the transition from n to m is given by

$$I_{n,m}(s) = a_{mn}^2 \left| \int \psi_n \psi_m^* \, e^{i\bar{s}\cdot\bar{r}} \, dv \right|^2 \tag{27}$$

$$a_{mn} = \omega'/\omega$$

where $\omega' = \omega - \omega_{mn}$ is the frequency of the scattered radiation and is now no longer the same as that of the incident radiation.

The total incoherent scattering intensity is obtained by summing over all $m \neq n$. Thus,

$$I_{inc}(s) = \sum_{n \neq m} I_{n,m}(s) = \sum_{n \neq m} a_{nm}^2 |f_{m,n}(s)|^2 \tag{28}$$

where $f_{m,n}(s)$ is the scattering factor associated with the transition from n to m.

The total scattered intensity, including that of the coherent radiation, is to be obtained by summing (28) over all values of m including n

$$I(s) = I_{coh}(s) + I_{inc}(s) = \sum_{m} a_{mn}^2 \left| \int \psi_m^* \psi_n \, e^{i\bar{s}\cdot\bar{r}} \, dv \right|^2 \tag{29}$$

This result is due to Wentzel[26].

C. The Many-Electron Atom

Let the suffix k refer to the coordinates of electron k in the atom. The wavefunction Φ is now a function of the time and all of the electron coordinates, 3Z in number, if the atom contains Z electrons.

The appropriate form of the wave equation is now

$$\sum_k \{ [\frac{-\hbar^2}{2m} \nabla_k^2 + V_k(r)]\Phi + \frac{i\hbar e}{mc} (\overline{A}_k \cdot \overline{\nabla}_k \Phi) \} = i\hbar \frac{\partial \Phi}{\partial t} \tag{30}$$

The wave functions corresponding to the stationary states of the unperturbed atom are of the type

$$\Phi_n = \psi_n(\overline{r}_1, \overline{r}_2, \cdots, \overline{r}_z)\ e^{-i\varepsilon_n t/\hbar}$$

where ψ_n is a function of the coordinates of all the electrons, given by $\overline{r}_1, \overline{r}_2, \cdots, \overline{r}_z$, and ε_n is the energy of the state n .

The quantity $|\Phi_n|^2 dv_1, dv_2, \cdots, dv_z$ gives the probability that electron $\{1\}$ lies within the element of volume dv_1 at the distance $\overline{r}_1$, electron $\{2\}$ within dv_2 at $\overline{r}_2$, etc. for the atom in state n . Then the charge density associated with the electron $\{k\}$ may be written as

$$\rho_k = e \int |\Phi_n|^2\ d'v_k \tag{31}$$

where $d'v_k$ denotes that the integration is over all electron coordinates except those of $\{k\}$. This integral gives the probability that the electron $\{k\}$ lies within the element of volume dv_k at $\overline{r}_k$ while the remaining electrons are anywhere and so is in a sense a measure of the average charge density at $\overline{r}_k$ due to electron $\{k\}$. By a method analogous to that given in I.B.1 it can be shown that ρ_k obeys the equation of continuity

$$\text{div}\ \overline{J}_k + \frac{\partial \rho_k}{\partial t} = 0 \tag{32}$$

where $\overline{J}_k$ is the current density associated with electron $\{k\}$ and is the expression (21) integrated over all electron coordinates except those of $\{k\}$.

Accepting this identification, the appropriate scattering factor for coherent radiation from a many-electron atom in the state n is, by analogy with (24),

$$f_{n,n}(s) = \sum_k \int |\Phi_n|^2 \, dv_k' \, e^{i\bar{s}\cdot\bar{r}_k} \, dv_k = \int |\Phi_n|^2 \sum_k e^{i\bar{s}\cdot\bar{r}_k} \, dv \qquad (33)$$

The expression for the total scattering intensity, coherent and incoherent, for an atom initially in the state n is

$$I(s) = \sum_m a_{mn}^2 \; \langle n|Q|m\rangle \; \langle m|Q^*|n\rangle \qquad (34)$$

where

$$\langle n|Q|m\rangle = \int \Phi_n^* \, \Phi_m Q \, dv \qquad (35)$$

$$Q = \sum_k e^{i\bar{s}\cdot\bar{r}_k} \qquad (36)$$

The summation in (34) is over all electronic states m for which the energy differences $\varepsilon_m - \varepsilon_n$ are less than the energy of the incident radiation.

1. Wavefunction

Generally, it is impossible to obtain exact solutions for the wavefunction Φ_n which satisfies the many-electron atom wave equation (30). As an approximation, the many-electron atomic wavefunction is assumed to be expressible as a product of Z one-electron wavefunctions. Since there is no means by which particular electrons may be identified, every possible permutation must be included. Further, Pauli's principle must be satisfied. The result, obtained by Slater[29], may be written as a determinant of Z rows and Z columns

$$\Phi_n = \begin{vmatrix} \psi_1(1) & \psi_1(2) \cdots \psi_1(z) \\ \vdots & \\ \psi_z(1) & \psi_z(2) \cdots \psi_z(z) \end{vmatrix} \Big/ \sqrt{Z!} \qquad (37)$$

The ψ_i are normalized and include spin orbitals.

Once the form of the wavefunction has been determined, the solution is obtained by some technique such as the self-consistent field method or variational technique[†].

2. Scattering Factors

If a wavefunction of the type (37) is used in (33), the scattering factor takes on the form

$$f_{n,n}(s) = \sum_k \int |\psi_k|^2 \, e^{i\bar{s}\cdot\bar{r}_k} \, dv_k = \sum_k f_k(s) \qquad (38)$$

The total atomic scattering factor is the sum of the scattering factors corresponding to the individual wavefunctions which the electrons occupy.

The expression for the total scattering, eq. (34), first given by Waller and Hartree[31], becomes

$$I(s) = Z + \sum_{j\neq k} f_j(s)\, f_k^*(s) - \sum_{j\neq k} |f_{jk}(s)|^2 \qquad (39)$$

[†] For details, see Offenhartz[30].

where

$$f_{jk}(s) = \int \psi_j^*(\bar{r}_p)\ \psi_k(\bar{r}_p)\ e^{i\bar{s}\cdot\bar{r}_p}\ dv_p \tag{40}$$

The quantity $f_{jk}(s)$ will usually be small, since $\psi_j(\bar{r}_p)$ is generally small in those regions where $\psi_k(\bar{r}_p)$ is large and vice-versa. Noting that $|\sum_k f_k(s)|^2$ may be written as

$$\sum_k |f_k(s)|^2 + \sum_{j\neq k} f_j(s)\ f_k^*(s)$$

the coherent and incoherent intensity are expressible in terms of the scattering factor as

$$I_{coh}(s) = |\sum_k\ f_k(s)|^2 \tag{41}$$

$$I_{inc}(s) = \sum_k\ \{1 - |f_k(s)|^2\} - \sum_{j\neq k} |f_{jk}(s)|^2 \tag{42}$$

The last term in (42) occurs because in a many-electron atom a number of electron levels are occupied. When the two electrons associated with the wavefunctions have the same spin, Pauli's principle applies, i.e., if the spins of the two electrons are the same they cannot occupy the same space wavefunction. When the spins are opposite there is nothing to prevent their doing so. For electrons with the same spin the space wavefunction is written as the determinant above. For electrons of opposite spins the wavefunction is symmetric in electron coordinates and the extra term in (42) does not appear. Thus, the summation in the last term is over all pairs of different electrons with the same spin.

D. Molecules

The unperturbed Hamiltonian for each N-nuclei and n-electron problem takes on the form[34]

$$H_I = \sum_i h(i) + (1/2) \sum_{i \neq j} e^2/r_{ij} \tag{43}$$

where the second summation represents the electrostatic interaction between electrons i and j at a distance r_{ij} ; i and j range from 1 to n ; $h(i)$ is the one-electron Hamiltonian operator for electron i and has the form

$$h(i) = -\frac{\hbar^2}{2m} \nabla_i^2 + V(i) \tag{44}$$

$V(i)$ is the potential energy of electron i in the presence of the fixed nuclei and has the form

$$V(i) = -\sum_{p=1}^{N} Z_p e^2 / r_{pi} \tag{45}$$

$Z_p e$ is the charge of the nucleus p and r_{pi} is the distance between electron i and the position of nucleus p .

Making the same assumptions for the wavefield as in I.B, the Hamiltonian of a molecular system, perturbed by a wavefield, becomes

$$H = H_I + \sum \frac{i\hbar e}{mc} \overline{A}_j \cdot \overline{\nabla}_j \tag{46}$$

This has the same form as the Hamiltonian of eq. (30) except for additional terms in H_I which arise due to the presence of more than one nucleus.

A determinantal form of the wavefunction may be chosen and the solution obtained by the self-consistent or variational method[34]. With this form of the wavefunction it can be shown that the resultant scattering factor for a molecule reduces to a summation of scattering factors over the electrons in the molecule[32].

E. Scattering by Liquids with Complex Molecules

The expressions derived below follow the treatment by Menke as discussed by James[32].

The scattering sample consists of N identical scattering molecules, each composed of n atoms. The different molecules are denoted by $\mu, \nu, \cdots$ and the individual atoms are labelled $p, q, \cdots$ within a molecule. Corresponding points in each molecule are chosen as molecular centers[†]. For the atom p in molecule μ, let

$$\bar{r}_{\mu p} = \bar{R}_{\mu} + \bar{v}_{\mu p} \tag{47}$$

where $\bar{r}_{\mu p}$ is a vector to the atom p in molecule μ from some convenient reference point O; $\bar{R}_{\mu}$ locates the molecular center of molecule μ, and $\bar{v}_{\mu p}$ is the vector from this molecular center to atom p within the molecule.

The amplitude scattered by molecule μ is given by

[†] As de Vries[33] has shown, the treatment being given here produces intensities which are not independent of the choice of molecular center. This of course does not correspond with reality. However, this analysis is sufficient for the purposes of succeeding sections, since only monatomic molecules will be considered. Otherwise, the expansions of Steele and Pecora[22] or Blum and Torruela[23] must be resorted to for proper description of the problem.

$\sum_p f_p(s)e^{i\bar{s}\cdot\bar{r}_{\mu p}}$ and the total amplitude scattered by the system is $\sum_\mu \sum_p f_p(s)\, e^{i\bar{s}\cdot\bar{r}_{\mu p}}$, the summation over p being over all the atoms in a molecule and over μ to include all the molecules.

The instantaneous coherent intensity, when (43) is used, is given by

$$I(s) = \sum_{\mu,p} \sum_{\nu,q} f_p(s)\, f_q^*(s)\, e^{i\bar{s}\cdot(\bar{R}_\mu - \bar{R}_\nu)}\, e^{i\bar{s}\cdot(\bar{v}_{\mu p} - \bar{v}_{\nu q})}$$

To obtain the observed intensity, this expression must be averaged over all possible orientations of the individual molecules, and all possible intermolecular distances. There are two types of terms to be considered: $\mu = \nu$, corresponding to internal interference effects, and $\mu \neq \nu$ corresponding to external effects. Terms of the first type, upon averaging and summing over all the molecules, lead to the expression

$$\bar{I}_i(s) = N\Big\{ \sum_p f_p^2(s) + 2 \sum_{p,q} f_p(s)\, f_q^*(s)\, \frac{\sin(s\ell_{pq})}{s\ell_{pq}} \Big\} \tag{49}$$

where ℓ_{pq} is the distance between atoms p and q in the same molecule.

Terms of the second type refer to atoms lying in different molecules. The vector $\bar{R}_{\mu\nu} = \bar{R}_\mu - \bar{R}_\nu$ is the vector distance between the reference centers of the two molecules. Consider $g(\bar{R}_{\mu\nu})dv_\mu dv_\nu/V^2$ to be the probability that the center of molecule μ lies in the element of volume dv_μ at a vector distance $\bar{R}_\mu$ from 0, while at the same time the center of molecule ν lies in dv_ν at a vector distance $\bar{R}_\nu$. V is the total volume of the sample and $g(\bar{R}_{\mu\nu})$ is the radial distribution function. Suppose $g(\overline{R}_{\mu\nu})$ to be the same for any pair of different molecules and to be spherically symmetric on the average. Neglecting the zero order maximum, the averaged scattering intensity is

$$\overline{I}_e(s) = F_e \frac{4\pi N}{V} (N-1) \int_0^\infty \{g(R) - 1\} R^2 \frac{\sin sR}{sR} dR \tag{50}$$

where

$$F_e = \sum_{p,q} f_p(s) f_q(s) \frac{\sin s\ell_{cp}}{s\ell_{cp}} \frac{\sin s\ell_{cq}}{s\ell_{cq}} \tag{51}$$

The scattering amplitude $f_p(s)$ has been assumed to be real. ℓ_{cp} is the distance of the atom of type p from the molecular center.

For monatomic molecules, the total averaged intensity per atom, $\overline{I}_i + \overline{I}_e$, reduces to

$$\overline{I}/N = f^2(s) \{1 + 4\pi\rho_o \int_0^\infty R^2[g(R) - 1] \frac{\sin sR}{sR} dR\} \tag{52}$$

where it has been assumed that the sample consists of identical atoms. $\rho_o = N/V$ is the average macroscopic density of the liquid and $N >> 1$.

Chapter II - Theory of X-Ray Scattering from Correlated Molecular Liquids

A. General Considerations

The scattering systems, considered in Chapter I, assumed the individual molecules to be fixed and far removed from each other. The validity of this model was established by Born and Oppenheimer[36] and a more general discussion was given by Born and Huang[37]. The total molecular wavefunction was expanded in terms of products of electronic and nuclear wavefunctions. The electronic wavefunction is a solution of Schrodinger's equation with the Hamiltonian operator given by (43). The nuclear wavefunction is derived from a nuclear eigenvalue equation in which the electronic energy, obtained from the solution of the electronic wave equation, occurs as a potential function. The admissibility of first solving the purely electronic problem rests on the large ratio between the electronic and nuclear masses.

At present, there is no model which gives a good approximation to the liquid state[†]. However, all of the existing models admit that the liquid state is somewhere in between the two extreme states of matter, solid and gas. Unlike these, in liquids both the atomic bindings and thermal motions are important, In addition, molecules in a liquid are constantly interacting with many of its neighbors. Depending upon

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[†] A "good model" is defined by Egelstaff[35] as one that would cover structural and thermal properties with equal emphasis.

the nature of the component molecules, i.e., whether they are ionic, the polarizability, the presence of induced and permanent dipoles, etc., their charge distributions are dependent on the local environment and, in general, upon configurations of the system.

To obtain the proper scattering intensity from such a system, the effects of molecular motion have to be included in the Hamiltonian operator. The corresponding wavefunction is then dependent on both electronic and nuclear coordinates. The result from such a calculation would be more accurate but the solution of such a many-body problem is intractable at present. Instead, as discussed in succeeding sections, a different approach is taken to include the many-body effect.

B. Effective Scattering Factors

The tack to be taken here is similar to McWeeny's[16] for obtaining the effective factor of atoms which bind to form molecules. The idea is extended to include any interacting system, whether binding or not.

1. Scattering Factors for Atoms in Molecules

McWeeny used the concept of "atomic" and "mobile" charge density to derive an expression for an effective scattering factor $f^e(s)$. The contribution to the effective factor, associated with the τ^{th} group of molecular orbitals, is

$$f_\mu(\tau) = q_\mu^\tau \int \rho_\mu^\tau \, e^{i\bar{s}\cdot\bar{r}_\mu} \, d\bar{r}_\mu + \sum_{\mu\neq\nu} \frac{1}{2} q_{\mu\nu}^\tau \int \rho_{\mu\nu}^\tau \, e^{i\bar{s}\cdot\bar{r}_\mu} \, d\bar{r}_\mu$$

$$= q_\mu^\tau f_\mu(\rho_\mu^\tau) + \frac{1}{2} \sum_{\mu\neq\nu} q_{\mu\nu}^\tau f_\mu(\rho_{\mu\nu}^\tau) \qquad (53)$$

where q_μ^τ and $q_{\mu\nu}^\tau$ measure respectively the amount of mobile charge associated with the atom μ and in the bond μ-ν , and

$$q_\mu^\tau = \sum_j X_{\mu j}^2 \tag{54}$$

$$q_{\mu\nu}^\tau = 2s_{\mu\nu} \sum_j X_{\mu j}\, X_{\nu j} \tag{55}$$

$f_\mu(\rho_\mu^\tau)$ is the scattering factor for an electron in the atomic orbital ϕ_μ ; $f_\mu(\rho_{\mu\nu}^\tau)$ is a bond scattering factor for bond μ-ν referred to atom μ ; $s_{\mu\nu}$ is the overlap between orbitals μ,ν . In this approach the molecular one-electron wavefunction is given by

$$\psi_j = \sum_\mu X_{\mu j}\, \phi_\mu \tag{56}$$

where the ϕ_μ are orbital functions centered at μ . Considering the effect of bonding as a correction, it is deduced that

$$f_\mu^e(s) = f_\mu^o(s) + \Delta f_\mu(s) \tag{57}$$

where $f_\mu^o(s)$ is the scattering factor for the isolated atom and the correction $\Delta f_\mu(s)$ is given by

$$\Delta f_\mu(s) = \sum_\tau (q_\mu^\tau - n_\mu^\tau)\, f_\mu(\rho_\mu^\tau) + \frac{1}{2} \sum_{\mu \neq \nu} q_{\mu\nu}^\tau\, f_\mu(\rho_{\mu\nu}^\tau) \tag{58}$$

n_μ^τ is the number of electrons originally on atom μ which go into the τ^{th} set of molecular orbitals. In general, the scattering factors are complex quantities.

The coefficients q_μ^τ and $q_{\mu\nu}^\tau$ may vary widely according to the molecular environment. These coefficients, therefore, determine the effective scattering factor in any given environment in terms of $f_\mu(\rho_\mu^\tau)$ and $f_\mu(\rho_{\mu\nu}^\tau)$ which are, to a first approximation, independent of the mobile electronic structure.

2. Instantaneous Scattering Factors and Molecular Correlations

The liquid sample is taken to consist of identical molecules. For a given isolated molecule in this liquid, the method of section II.B.1 is used to compute the scattering factor, which is the scattering factor for the isolated molecule.

In section I.D it was shown that for a certain form of the wavefunction the scattering factor for a molecule is the sum of the scattering factors for the individual molecular orbitals. It will be assumed that this is still the case in the following discussion, thus confining it to orbitals.

Consider the liquid to consist of a sea of molecules, all moving randomly and interacting with one another. In some cases, depending upon the proximity of the molecules and their character, there may be a flow of charge between them, or they may just suffer distortions of their charge density distribution, or both.

Suppose $\Delta f_p^k(s,\bar{r}_k)$ is the orientationally dependent correction, at some instant, due to pairwise interaction between the p^{th} and k^{th} molecules, a reference point in the latter being located at a distance $\bar{r}_k$ from a similar reference point in the former. $\Delta f_p^{kj}(s,\bar{r}_j,\bar{r}_k)$ is the orientationally dependent correction arising from triplet interactions, with molecules j and k distant $\bar{r}_j$ and $\bar{r}_k$ from the p^{th}, and similarly for higher order terms. Let $\bar{R}$ be the set of all $\bar{R}_i$

specifying the instantaneous configuration of the molecules; then, the instantaneous value of the scattering factor for a given orbital in the p^{th} molecule is to be written

$$f_p(\overline{R},s) = f_p^o(s) + \sum_k \Delta f_p^k(s,\overline{r}_k) + \sum_{j,k} \Delta f_p^{kj}(s,\overline{r}_j,\overline{r}_k) + \cdots \tag{59}$$

where $f_p^o(s)$ is the scattering factor for the given orbital in the isolated molecule p . k and j range from 1 to $N-1$, $k \neq p$, $j \neq p$.

Note that by definition

$$\Delta f_p^p(s,\overline{r}_p) \equiv 0 \tag{60}$$

$$\Delta f_p^{kk}(s,\overline{r}_k,\overline{r}_k) \equiv 0 \tag{61}$$

$$\Delta f_p^{pp}(s,\overline{r}_p,\overline{r}_p) \equiv 0 \tag{62}$$

The summations in (59) can thus be extended to include all the molecules.

The instantaneous scattering factor for the p^{th} molecule is given by summing (59) over all the orbitals which contain electrons. This quantity is dependent both on the molecular orientations and configurations.

3. Evaluation of the Correlation Terms

A possible way of evaluating the correlation terms in some convenient coordinate system is given below.

$\Delta f_p^k(s,\overline{r}_k)$ is found by evaluating the scattering factor for two interacting molecules separated at a distance $\overline{r}_k$. The value of the isolated molecules scattering factor, when the two molecules are at the same distance from each other, is known. Subtraction of the latter from the former yields the desired result.

For the triplet term the molecular scattering factor is evaluated for the given configuration of $\bar{r}_j, \bar{r}_k$. For the same configuration the isolated molecules scattering factor is computed. The value of the three pairwise correlation terms is also computed for this configuration. Subtracting the latter two results from the first gives the triplet correlation. This process may be extended to higher order terms.

C. Coherent Scattering from a Liquid

The instantaneous coherent scattering intensity, when the correlation terms are included, is given by an equation similar to (48),

$$I(s) = \sum_{p,q} f_p(\bar{R},s)\, f_q^*(\bar{R},s)\, e^{i\bar{s}\cdot(\bar{R}_p - \bar{R}_q)} \tag{63}$$

Using (59) - (62), the instantaneous intensity may be written

$$\begin{aligned} I(s) = \sum_{p,q} & \{f_p^o(s) + \sum_m \Delta f_p^m(s,\bar{r}_m) + \sum_{k,j} \Delta f_p^{kj}(s,\bar{r}_k,\bar{r}_j) + \cdots\} \\ & \times \{f_q^{o*}(s) + \sum_n \Delta f_q^{n*}(s,\bar{r}_n) + \sum_{i,t} \Delta f_q^{it*}(s,\bar{r}_i,\bar{r}_t) + \cdots\}\, e^{i\bar{s}\cdot\bar{R}_{pq}} \end{aligned} \tag{64}$$

Retaining the pairwise interaction terms only, (64) may be written as a sum of four terms,

$$I_1(s) = \sum_{p,q} f_p^o(s)\, f_q^o(s)^*\, e^{i\bar{s}\cdot\bar{R}_{pq}} \tag{65}$$

$$I_2(s) = \sum_{p,q,n} f_p^o(s)\, \Delta f_q^{n*}(s,\bar{r}_n)\, e^{i\bar{s}\cdot\bar{R}_{pq}} \tag{66}$$

$$I_3(s) \quad \sum_{p,q,m} f_q^o(s)^*\, \Delta f_p^m(s,\bar{r}_m)\, e^{i\bar{s}\cdot\bar{R}_{pq}} \tag{67}$$

$$I_4(s) = \sum_{p,q,m,n} \Delta f_p^m(s,\bar{r}_m)\, \Delta f_q^{n*}(s,\bar{r}_n)\, e^{i\bar{s}\cdot\bar{R}_{pq}} \tag{68}$$

where $\bar{R}_{pq} = \bar{R}_p - \bar{R}_q$

1. Orientational Average

For molecules which do not possess spherical symmetry the configuration of pairs of molecules is given by a vector $\bar{R}$ and the three Euler angles $\bar{\Omega} = (\alpha,\beta,\gamma)$. The molecular pair correlation function has the form $g(\bar{R},\bar{\Omega})$. In general, $g(\bar{R},\bar{\Omega})$ cannot be obtained from scattering of a liquid since the data is usually one-dimensional.

It will be assumed in the following that the orientation of pairs of molecules is independent of their separation. Thus $g(\bar{R},\bar{\Omega})$ may be written as $g(\bar{R}) \cdot g(\bar{\Omega})$ and further, if the sample has macroscopic isotropy, $g(\bar{\Omega}) = 1$. Bars over the appropriate variables indicate orientational average. Then

$$\bar{I}_1(s) = \sum_{p,q} f_p^o(s)\, f_q^o(s)^*\, \overline{e^{i\bar{s}\cdot\bar{R}_{pq}}} \tag{65a}$$

where

$$\overline{e^{i\bar{s}\cdot\bar{R}_{pq}}} = \int_0^{\pi} e^{isR_{pq}\cos t} \frac{1}{2}\sin t\, dt = \frac{\sin(sR_{pq})}{(sR_{pq})} \tag{69}$$

Since m is a dummy index, $I_3(s)$ may be rewritten in the form

$$I_3(s) = \sum_{p,q,n} f_q^o(s)^* \, \Delta f_p^n(s,\bar{r}_n) e^{i\bar{s}\cdot\bar{R}_{pq}}$$

$$= \sum_{p,q,n} [f_q^o(s) \, \Delta f_p^n(s,\bar{r}_n)^* e^{-\bar{s}\cdot\bar{R}_{pq}}]^* \tag{70}$$

Similarly, p and q may be interchanged,

$$I_3(s) = \sum_{p,q,n} [f_p^o(s) \, \Delta f_q^n(s,\bar{r}_n)^* \, e^{i\bar{s}\cdot\bar{R}_{pq}}]^* = I_2(s)^* \tag{70a}$$

Assuming that $f_p^o(s)$ is real,

$$I_{32}(s) = I_3(s) + I_2(s) =$$

$$= 2 \sum_{p,q,n} f_p^o(s) \, \mathrm{Re} \, \{\Delta f_q^n(s,\bar{r}_n)^* \, e^{i\bar{s}\cdot\bar{R}_{pq}}\} \tag{71}$$

In the above summation several different types of terms may be identified: a) $p = q$, due to internal interference between the isolated q^{th} molecular charge distribution and the correlation charge density within it that arises from the presence of a second molecule, the n^{th}; b) $p = n$, $p \neq q$, due to external interference between the p^{th} isolated molecular charge distribution and the correlation charge density it creates within the q^{th} molecule; c) $p \neq q$, $p \neq n$, external interference between an isolated charge density p^{th} and a correlation charge density q^{th} , the latter being produced by the presence of a third, the n^{th}, molecule.

With the assumption that the orientation of pairs of molecules is independent of their separation,

$$\overline{I}_{32}(s) = \overline{I}_a + \overline{I}_b + \overline{I}_c \tag{72}$$

$$\overline{I}_a = 2 \sum_{p,n} f_p^o(s)\ \overline{F}_p^n(s,\overline{r}_n) \tag{73}$$

$$\overline{I}_b = 2 \sum_{p,q} f_p^o(s)\ \overline{F}_q^p(s,\overline{r}_p) \tag{74}$$

$$\overline{I}_c = 2 \sum_{p,q,n} f_p^o(s)\ \overline{F}_q^n(s,\overline{r}_n) \tag{75}$$

where the averages within the respective sums are given by

$$\overline{F}_p^n(s,r_n) = \frac{1}{2}\int_0^{\pi} \mathrm{Re}\{\Delta f_p^n(s,\overline{r}_n)^*\}\ \sin\alpha\ d\alpha \tag{76}$$

$$\overline{F}_q^p(s,r_p) = \frac{1}{2}\int_0^{\pi} \mathrm{Re}\{\Delta f_q^p(s,r_p)^*\ e^{isR_{pq}\cos\alpha}\}\ \sin\alpha\ d\alpha \tag{77}$$

$$\overline{F}_q^n(s,r_n) = \frac{1}{4}\int_0^{\pi}\int_0^{\pi} \mathrm{Re}\{\Delta f_q^n(s,\overline{r}_n)^*\ e^{isR_{pq}\cos\beta}\}\sin\beta\ \sin\alpha\ d\alpha d\beta \tag{78}$$

It is implicitly understood that $\Delta f_p^q(s,\overline{r}_p)$ is a function of the orientation angle α between the scattering vector $\overline{s}$ and the imagined axis joining corresponding reference points in the molecular pair. Similarly, β is the orientation of $\overline{s}$ relative to R_{pq} when there are three molecules.

If the highest symmetry of an orbital is that of a p-type function, the result deduced by McWeeny[15]

$$f = f(s,\alpha=0)\ \cos^2\alpha + f(s,\alpha=\tfrac{\pi}{2})\sin^2\alpha \tag{79}$$

may be used. Using this functional form for the correlation scattering factor term, the orientational average for the three different cases (73)-(75) results in

$$\overline{F}^n_p(s,\overline{r}_n) = (1/2)\int_0^\pi \mathrm{Re}\{\Delta f(\alpha,s)\}\ \sin\alpha\ d\alpha \tag{80}$$

$$\overline{F}^p_q(s,\overline{r}_p) = (1/2)\int_0^\pi \mathrm{Re}\{\Delta f(\alpha,s)e^{isR_{pq}\cos\alpha}\}\sin\alpha\ d\alpha \tag{81}$$

$$\overline{F}^n_q(s,\overline{r}_n) = (1/4)\int_0^\pi\int_0^\pi \mathrm{Re}\{\Delta f(\alpha,s)e^{isR_{pq}\cos\beta}\}\sin\beta\sin\alpha\ d\alpha\ d\beta \tag{82}$$

where

$$\Delta f(\alpha,s) = \Delta f^j_i(s,\overline{r}_j,\alpha=0)^*\cos^2\alpha + \Delta f^j_i(s,\overline{r}_j,\alpha=\pi/2)^*\sin^2\alpha \tag{83}$$

The indices i and j take on the appropriate values as the corresponding indices on the left hand side of equations (80)-(82).

When the analytic form (83) is used for the correlation scattering factor term, the orientational averages specified by eqs. (80)-(82) may be written explicitly

$$\overline{F}^n_p(s,\overline{R}_n) = \mathrm{Re}\{\Delta f^n_p(s,\overline{R}_n,\alpha=0)^* + 2\Delta f^n_p(s,\overline{R}_n,\alpha=\tfrac{\pi}{2})^*]\}\ /\ 3 \tag{84}$$

$$\begin{aligned}\overline{F}^p_q(s,\overline{R}_p) = \mathrm{Re}\Bigg\{&\Delta f^p_q(s,\overline{R}_p,\alpha=0)^*\left[\frac{\sin(sR_p)}{sR_p} + \frac{2\cos(sR_p)}{(sR_p)^2} - \frac{2\sin(sR_p)}{(sR_p)^3}\right]\\ &+ \Delta f^p_q(s,\overline{R}_p,\alpha=\tfrac{\pi}{2})^*\left[\frac{2\sin(sR_p)}{(sR_p)^3} - \frac{2\cos(sR_p)}{(sR_p)^2}\right]\Bigg\}\end{aligned} \tag{85}$$

$$\overline{F}^p_q(s,\overline{R}_p,\overline{R}_n) = (1/3)\mathrm{Re}\{\Delta f^p_q(s,\overline{R}_p,\alpha=0)^* + 2\Delta f^p_q(s,\overline{R}_p,\alpha=\tfrac{\pi}{2})^*\}\ \frac{\sin(sR_n)}{(sR_n)} \tag{86}$$

2. Configurational Average

It remains to average the results of the previous section over all the different configurations the system may take. Brackets denote configurationally averaged quantities.

The result $\overline{I}_1(s)$ given by eq. (65a) may be split into two terms, for which $p = q$ and $p \neq q$ respectively. This may then be written

$$\overline{I}_1(s) = \sum_p f_p^o(s)^* + \sum_{p\neq q} f_p^o(s)\, f_q^o(s)^* \frac{\sin(SR_{pq})}{(SR_{pq})} \tag{87}$$

Using the distribution function defined in section I.D., the averaged intensity, excluding zero-order scattering, is

$$\langle\overline{I}_1(s)\rangle = \sum_p f_p^o(s)f_p^o(s)^* + \sum_{p\neq q} f_p^o(s)f_q^o(s)^* \cdot \frac{4\pi}{V} \int [g(R_{pq})-1] \frac{\sin(sR_{pq})}{S} R_{pq}\, dR_{pq} \tag{88}$$

If all the molecules are identical, each term within the summation yields the same average, thus

$$\overline{I}_1(s) = Nf_p^o(s)f_p^o(s)^* + N(N-1)f_p^o(s)f_q^o(s)^* \frac{4\pi}{V} \int [g(R)-1]\frac{R}{S}\cdot\sin(SR)\,dR \tag{89}$$

The subscripts have been purposely left in to indicate that two different isolated molecules are involved in the second term of (89).

If $\rho_o = N/V$, and $N >> 1$,

$$\langle\overline{I}_1(s)\rangle = N[f_p^o(s)f_p^o(s)^* + f_p^o(s)f_q^o(s)^* 4\pi\rho_o \int [g(R)-1]R\,\sin(SR)dR/S] \tag{90}$$

This is the Zernike-Prins relation. It is a simple procedure to show that this reduces to the form of expressions (49) and (50), when the molecular scattering amplitude is assumed to be given by a sum over the individual atoms forming the molecule. The result of this exercise is given in section I.D. If the molecules are monoatomic, eq. (52) is obtained.

Next, consider $\overline{I}_{32}(s)$ which consists of a sum of the three terms $\overline{I}_a$, $\overline{I}_b$, $\overline{I}_c$.

The average for $\overline{I}_a$ is given by

$$\langle\overline{I}_a\rangle = 2\sum_{p,n} f_p^o(s) \int \overline{F}_p^n(s,R_n)g(R_{pn})dV_p dV_n/V^2 \tag{91}$$

Transforming to relative coordinates,

$$\langle\overline{I}_a\rangle = 2\sum_{p,n} f_p^o(s) \int \overline{F}_p^n(s,R_n)g(R_n)dV_n/V \tag{92}$$

The integrals within the summation are the same. Using the same assumptions as for (90),

$$\langle\overline{I}_a\rangle = 2N\rho_o f_p^o(s) \int \overline{F}_p^n(s,R_n)g(R_n)dV_n \tag{93}$$

Similarly, the average for $\overline{I}_b$ is

$$\langle\overline{I}_b\rangle = 2\sum_{p,q} f_p^o(s) \int \overline{F}_q^p(s,R_p)g(R_{pq})dV_p dV_q/V^2 \tag{94}$$

or in relative coordinates, when the sum is performed,

$$\langle\overline{I}_b\rangle = 2N\rho_o f_p^o(s) \int \overline{F}_q^p(s,R_p)g(R_p)dV_p \tag{95}$$

The configurational average for $\bar{I}_c$ depends upon the different arrangement of three particles. Thus, the resultant average must be expressed in terms of the triplet correlation function $\rho^3(\bar{R}_p,\bar{R}_q,\bar{R}_n)$, and has the form

$$\langle\bar{I}_c\rangle = 2 \sum_{p,q,n} f_p^o(s) \int \bar{F}_q^n(s,\bar{R}_n)\rho^3(\bar{R}_p,\bar{R}_q,\bar{R}_n)dV_p dV_q dV_n \qquad (96)$$

Invoking the superposition approximation, and expressing the result in terms of the radial distribution functions,

$$\langle\bar{I}_c\rangle = 2 \sum_{p,q,n} f_p^o(s) \int \bar{F}_q^n(s,R_n) g(R_{pq}) g(R_{pn}) g(R_{qn}) dV_p dV_q dV_n / V^3 \qquad (97)$$

The average will be the same for any triple of molecules. Performing the sum, the expression becomes,

$$\langle\bar{I}_c\rangle = 2N\rho_o^2\, f_p^o(s) \int \bar{F}_q^n(s,R_n) g(R_{pn}) g(R_{pq}) g(R_{qn}) dV_p dV_q dV_n \qquad (98)$$

and in relative coordinates,

$$\langle\bar{I}_c\rangle = 2N\rho_o^2 f_p^o(s) \int \bar{F}_q^n(s,R_n) g(R_n) g(R_p) g(R_{pn}) dV_p dV_n \qquad (99)$$

The total coherent intensity, when intermolecular correlations to the first order in $\Delta f_p^q(s,r_q)$ are included, is given by the sum of eqs. (90), (93), (95) and (96) or (99).

Specifically, for monoatomic molecules and when the superposition approximation is used, the total coherent intensity per atom is

$$\frac{I(s)}{N} = f^{o2}(s)\left[1+4\pi\rho_o\int(g(R)-1)R\ \sin SRdR/s\right] + \frac{\Delta I(s)}{N} \tag{100}$$

where

$$\frac{\Delta I(s)}{N} = 2f^{o}(s)[\rho_o\int[\overline{F}^{n}_{q}(s,R)+\overline{F}^{p}_{q}(s,R)]g(R)dV$$

$$+\rho_o^2\int\overline{F}^{n}_{q}(s,R_n)g(R_n)g(R_p)g(R_{pn})dV_p dV_n] \tag{101}$$

D. Incoherent Scattering from a Liquid

To arrive at the coherent scattering intensity, eq. (42) is used to calculate the amount of incoherent scattering to be subtracted from the total measured intensity. Consistent with the method of this chapter, the effects of intermolecular correlation have to be included.

Using notation similar as that for eq. (59), define the effective exchange scattering factor, between orbitals j and k in the μ^{th} particle as

$$f_{jk,\mu}(\overline{R},S) = f^{o}_{jk,\mu}(s) + \sum_{\nu}\Delta f^{\nu}_{jk,\mu}(s,R_\nu) + \ldots \tag{102}$$

where $f^{o}_{jk,\mu}(s)$ is the exchange scattering amplitude for the orbitals j,k in the μ^{th} isolated molecule (or atom), as computed by eq. (40. $\Delta f^{\nu}_{jk,\mu}(s,R_\nu)$ is the correlation term for the exchange scattering amplitude between the same orbitals in that particle, due to the presence of another particle ν at a distance R_ν. The correlation terms are computed in a manner identical to that discussed for the orbital scattering amplitudes in section II.B.3.

Placing eqs. (59) and (102) in (42), yields the instantaneous incoherent scattering intensity for a particle,

$$I_{inc}(s) = \sum_k [1-|f_k^o(s)|^2 - f_k^o(s) \sum_q 2\mathrm{Re}\{\Delta f_k^q(s,R_q)\}]$$

$$- \sum_{j\neq k} [|f_{jk,\mu}^o(s)|^2 + \overset{*o}{f}_{jk}(s) \sum_\nu 2\mathrm{Re}\{\Delta f_{jk,\mu}^\nu(s,R_\nu)\}] + \ldots \qquad (103)$$

The orientational average of the two correlation terms above are

$$\overline{F}_k^q(S,R_q) = (1/2) \int_o^\pi \mathrm{Re}\{\Delta f_k^q(s,R_q)\} \sin\alpha \; d\alpha \qquad (104)$$

and

$$\overline{F}_{jk,\mu}^\nu(s,R_\nu) = (1/2) \int_o^\pi \mathrm{Re}\{\Delta f_{jk,\mu}^\nu(s,R_\nu)\} \sin\alpha \; d\alpha \qquad (105)$$

where the correlations are implied functions of α, the orientation angle. Note that eqs. (104) and (105) are eq. (76) with $\Delta f_p^n(s,R_n)$ replaced by the appropriate correlation term from (103).

Configuration averaging (104) and (105), the final expression for the incoherent scattering per particle is

$$I_{inc}(s) = \sum_k \{1-|f_k^o(s)|^2 - f_k^o(s) \sum_q 2\int \overline{F}_k^q(s,R_q) g(R_q) dV_q/V$$

$$- \sum_{j\neq k} \{|f_{jk,\mu}^o(s)|^2 - f_{jk,\mu}^{o^*}(s) \sum_\nu 2\int \overline{F}_{jk}^\nu(s,R_\nu) g(R_\nu) dV_\nu/V\}$$

$$(106)$$

The sums over q,ν are over the different particles in the sample. For a monoatomic liquid, composed of identical atoms, all the terms are the same. Thus,

$$I_{inc}(s) = \sum_{k} \{1-|f_{k}^{o}(s)|^{2} - f_{k}^{o}(s)\rho_{o} < \overline{F}_{k}^{q}\ (s,R_{q})>\}$$

$$- \sum_{j\neq k} \{|f_{jk,\mu}^{o}(s)|^{2} - f_{jk,\mu}^{o\,\nu *}(s)\rho_{o} < \overline{F}_{jk,\mu}^{\nu}(S,R_{q})>\} \qquad (107)$$

where the brackets < > denote configurational average.

The total incoherent scattering intensity is obtained by multiplying the expression (107) by the number of scattering particles in the sample.

Equations (101) and (107) present the new results for X-ray scattering from a liquid. The additional terms are a consequence of the non-static nature of the structure and represent an average over all the possible (pairwise) configurations of the system. Its analogue in X-ray crystallography, thermal diffuse scattering by lattice vibrations has been studied quite extensively.[†]

[†] An up-to-date survey of the subject may be found in the book by Maradudin, Montroll, Weiss, and Ipatova.[38] From the crystallographers' viewpoint, James,[32] gives both theoretical and experimental discussions.

Chapter III

Computational Results

A. Procedure

The computations for hydrogen and some preliminary work for helium were done with the aid of an IBM 360/75 computer. The final calculations for helium and argon were performed on the IBM 370/155. Overlapping calculations for helium were used to determine the effects of changing machines. None were found.

The numerical accuracy of the program computing the scattering factors was checked in two ways. First, by comparison of isolated atom results from the molecular scattering factor program, with the results from an independent Hartree-Fock wavefunction program, using the method of Froese.[41] Second, where available, by setting $s = 0$, overlap integrals were compared with those listed for the wavefunction. The results agree to four decimal places.

The correlation terms were computed in the following way. Wavefunctions for the various intermolecular separations were supplied to the program. The effective scattering factor was then computed relative to the midpoint of the line connecting the intermolecular centers, since there the expressions are simplest. The non-interacting particle wavefunctions were also fed in and the value of the scattering factor determined relative to the same center for the given separations. To obtain the correlation, relative to each atomic or molecular center, the latter is subtracted from the former, the result is divided by two, and translated to the appropriate molecular or atomic center.

This number represents the correlation scattering factor and any further reference to correlation will be implicitly understood to arise from this quantity. Since the number of intermolecular points available was limited, cubic spline interpolation[39] was used for interpolation to produce smoothed curves. The correlation terms were then averaged over orientations and configurations as specified in Chapter II. The radial distribution function used for configuration averaging was obtained from experimental X-ray scattering data. Below, these results and the effects of correlation on the various computed quantities will be discussed.

B. Hydrogen

Computations for the molecular scattering factors of H_2 have been performed previously (McWeeny;[16] Stewart et al.[40]). The variation in the scattering amplitude as the two atoms unite does not exist in the literature. Moreover, the H-H system represents the simplest system, where, ignoring the presence of permanent dipoles, the interactions can be expected to be significant over considerably large distances of separation. This, and the availability of the scattering amplitudes at the equilibrium separation, made it an ideal starting point for this study. The wavefunction was obtained by Huestis.[45]

B.1 Scattering Plane Normal to Bond Axis

Figure 1 compares the instantaneous isolated atom scattering factor $f_p^o(s)$, and the instantaneous effective atomic scattering factor $f_p(R,s)$, i.e., the scattering factor as given by eq. (59) with $k = 1$.

Comparison of $f_p(R,s)$, given by curve 1, and $f_p^o(s)$, curve 3, shows marked differences in the former due to contraction and polarization of the charge distribution. At large separations, the corrections are quite small and negligible. They become more significant as the interatomic separation decreases. The decrease in the effective factor, as the atoms approach each other is attributable to charge leaking off from the atoms to form the bond. Simultaneously, the charge around each atom contracts. However, this is not sufficient to offset the loss of charge to the bond. Thus, there is a net decrease in the effective atomic scattering factor amplitude. This is best shown in fig. 2, where the variation of the effective factor vs. separation, for select values of X $(= \sin(\theta)/\lambda)$, is shown. For large separations the effective factor tends to the limiting value of the isolated atom. As the two atoms approach each other, there is no significant change until about 4 Å. For separations shorter than this, the interaction produces significant deviations. The separation is such that the overlapping of the orbitals produces an increase in the localized charge density. $f_p(R,s)$ now begins to rise in value. As X is increased, the rise in $f_p(R,s)$ begins to occur at progressively smaller separations. This is because an increase in X is the same as resolving the behavior for distances closer to the atom. This behavior is well portrayed in the plot of the magnitude of the corrections vs. R, fig. 3.

2. Scattering Plane Parallel to Bond Axis

Figure 4 shows the effective scattering factors when the scattering vector is normal to the bond axis. The behavior is similar to that of section III.B.1. In the present case, however, the effective values are closer to those of the isolated atom. The orientation of the scattering vector specifies the amount of interaction that occurs between the scatterer and the incident field (eqs. (1) and (13)). Since there is not much interaction along directions normal to the internuclear axis, the contraction of the orbital predominates the change to the scattering amplitude. Figure 5 shows the variation of the effective factor vs. R. The values remain essentially constant, except for distances close to equilibrium, where overlap effects become significant.

C. Helium

Appendix B.3 discusses the helium wavefunction.

The effective scattering factor for the outer orbital is computed on the basis of its change in character from an 1s type orbital to a sigma-u type, when two interacting He atoms approach each other. The effective scattering factor for the inner orbital is computed as described in section III.A.

1. Correlation Amplitudes

Figures 6 and 7 compare the correlation amplitudes vs. R for selected values of X, when the orientation of the scattering vector is parallel to the internuclear axis. Both sigma-g and sigma-u orbitals are shown. Tables 1 and 2 list these values. Figures 8 and 9 compare the same except the scattering plane is parallel to the internuclear axis. The values are listed in tables 3 and 4. It is immediately clear, from these plots, that the net change for the atom as a whole will be small, since the orbitals behave in opposite fashion. While the sigma-u orbital tends to expand, the sigma-g contracts as the atoms approach each other. For large values of X (scattering from the inner core), the correlation amplitudes are small, as would be expected, due to shielding from the outer charge.

The orientational average of the correlation terms, listed in tables 5 and 6, and shown in figs. 10 and 11, is of the same order of magnitude as the unaveraged terms. The tendency of the orbitals to counteract each other has not been destroyed.

Figures 12 and 13 show the behavior of the correlations when summed over all the orbitals (the net orbital correlation), and the ratio of the net correlation to the isolated atom scattering factor. These values are listed in tables 7 and 8. Noticeable effects take place at values of R less than 2.5 Å. This is the approximate value of σ, the hard sphere diameter for helium.[1] It may be noted that the minimum values of the ratio occur in the vicinity of separations for which the calculations of Lim and Linder[48] show a maximum in the polarizability.

C.2 Direct Correlation Function, Radial Distribution Function and Potential Energy

Using the experimental X-ray data for helium, obtained by

Gordon, Shaw and Daunt,[49] the effect of including correlations in the scattering data of two thermodynamic states, $T = 1.4^\circ K$, $\rho_o = .02178$ atoms/$\AA^3$ and $T = 4.2^\circ K$, $\rho_o = .01885$ atoms/$\AA^3$ was considered.

The structure factors, for the two states, and the appropriate correlation intensities are shown in figs. 14 and 15. The values are listed in table 9. It is apparent that the shape of the correlation intensity curve is not much different above or below the λ-transition temperature of liquid helium. However, at higher angles of scattering, the correlation intensity below the transition temperature is larger and the curve is broader due to closer packing. Thus, as one would expect, short range fluctuations are more significant.

The radial distribution functions, figs. 16 and 17, when correlations are included, become slightly broader and the first peak is about .1% lower.

The direct correlation function, $C(R)$, figs. 18 and 19, increases in magnitude by about 1% below the λ-temperature and about 2% above. This behavior is to be expected since at the higher temperature state there is more likelihood of the particles to be found at separations greater than the first peak value. Thus, short range fluctuations become significant at higher temperatures. On the scale of the figures, these effects are not detectable. Numerical values are listed in table 10.

No satisfactory theory exists to predict the energy of liquid helium. Murphy and Watts,[50] have shown that the hypernetted chain equation (HNC) yields more accurate results. Nevertheless, these are only semiquantitative in application to the liquid state (Feenberg[51]). Thus, assuming that the same deficiencies exist, whether the structure factor includes the correlation intensity or not, the difference in the potential for these two cases was calculated, for each state. The results are displayed in figs. 20 and 21 and table 10. Above the transition temperature, and in the vicinity of the equilibrium separation, the potential well is depressed by about 5%. Below the transition temperature the well is deeper by about 1%. In both cases it is broader.

D. Argon

Wavefunctions for interacting argon atoms, whose separations are greater than 2.6 Å were not available. Since the interactions beyond these separations are weak, the value of the effective factor was computed at this separation using the wavefunction for Ar_2 obtained by Gilbert and Wahl,[47] described in Appendix D.4.

The correlation amplitudes were calculated as described before. A straight line fit was used to interpolate for values at intermediate separations. Figure 22 shows a plot of the net correlations, orientationally averaged, and also their ratio to the scattering amplitude of an isolated atom. The order of magnitude of these correlations is the same as for He_2.

The X-ray data used for this study on argon is listed in table 11, and were obtained by Kirstein.[14]

The correlation intensities, for five thermodynamic states are shown in figs. 23 to 27. All have the same variation with scattering angle and the same order of magnitude except for the state at $T = 143^{0}K$ and $\rho_{o} = .91$ gm/cc. This state is at a higher temperature and considerably lower pressure than the other states, which are grouped within a narrow density region. This accounts for the lowered correlation intensity, which is state dependent through the radial distribution function.

The radial distribution function is plotted in figs. 28 through 32. There are no dramatic differences due to correlation. When the numerical values, table 12, are compared, the first peak of g(R) has been lowered 1% and has become slightly broadened.

The direct correlation function, figs. 33 to 37, since its integrand contains the structure factor in the numerator and denominator is more sensitive to correlations. The main peak is lowered by 5%. Away from the main peak, towards larger separations, there is an increase of about 2%.

The effect on the potential energy is displayed in figs. 38 to 42. Values of the potential are in table 12. The depth of the potential well has been lowered by about 5%. The width of the wells is considerably broadened.

E. Discussion

The calculations on hydrogen confirm the results of McWeeny.[15] Correlation effects due to bonding may be considerable. No further work was done on this system since in the liquid state hydrogen exists in the molecular form H_2 rather than as H.

The ground state of liquid He has been the subject of many studies (reference 51 contains a good compendium). In particular, the study conducted by Gordon et al.,[49] attempted to determine if there are any changes in the structure above and below the λ temperature. Their result shows that at temperatures below, it is slightly expanded due to the existence of a large zero point energy. When intermolecular correlations are accounted for, there is no change in this behavior. However, both below and above the transition temperature, the first peak is reduced by 1% and is broader.

A comparison of the difference in the potential energy shows that while the average structure is not affected much, the potential is depressed by 5%. Wang,[52] showed that the instantaneous polarization of one atom by another results in a correlation between the electron coordinates, and therefore in attraction. Massey and Woo[53] performed a calculation on the ground state of liquid He using correlated basis functions. Their results show that the potential energy is lower than for an uncorrelated basis.

The results for argon, expectedly, are very similar to those for helium. g(R) is broadened, and the peak value is decreased by the same order of magnitude. The correlation function, for large R, does not go to zero as fast, indicating that forces might be longer range than expected from previous experimental results. The potential is also more attractive and the well is broader. Rowlinson et al.[54] have studied the variation of the potential minima of argon as a function of density. Their results, deduced by including higher order interactions, also indicate that the potential well depths, obtained by X-ray scattering, should be lower.

Chapter IV

Conclusions and Recommendations

The results of this study show that the structure and intermolecular potential of a simple, weakly interacting liquid, when obtained from experimental X-ray scattering data, must include intermolecular correlations if there is to be any hope of obtaining a proper description of the sample.

At large scattering angles, where the data produces an apparent structure factor of zero, the correlations have not yet disappeared. Short range correlations are not negligible. Significantly, at these angles, the correlation amplitudes are within the error bars of present data. To get a representation for the effect of this deficiency, the data was deliberately truncated at a point where the sturcture is known not to be zero. Although quantitative agreement was not obtained, the same relative effects were observed in the properties. Thus, regardless of whether the structure factors represent the state properly, there is no question that it contains noise in the form of the correlations considered here. A more complete set would produce more accurate results.

It may prove fruitful to incorporate higher order correlation terms in the correlation amplitudes, especially since the work of Rowlinson et al.[54] shows lowered potential minima due to inclusion of these correlations.

Since molecular fluctuations become large in the vicinity of the critical region, it would be an interesting, and perhaps fruitful exercise, to analyse data in that region using the method that has been presented here.

There are other systems which should be considered. Liquid H_2O, which contains permanent dipoles, and substances which are mixtures. Liquid crystals, which possess a large polarizability and freedom of motion.

Treatments of thermal diffuse scattering, in solids, which assume isolated atomic or molecular charge distributions, are no longer acceptable.

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Appendix A

Scattering Factor Matrix Elements

As described in Appendix B, the scattering factors in this work utilize Slater-type orbitals expanded in terms of Gaussian functions. All p-type functions are assumed to be positive along the positive Z-axis, which points to the right. The X-Z plane is in the plane of the paper. Thus, the positive Y-axis points out of the plane of the paper. All integrals are performed at the midpoint of the internuclear axis, where the expressions are simplest. The axis is of length R. Below are listed the analytical integration results for the different types of functions used in the expansion. Subscripts L or R refer to functions which are centered on the left or right centers, respectively. p and q refer to the p^{th} and q^{th} functions of the given type. N_p and N_q are normalization constants.

$$N_p^2 = 1/ \int e^{-2\beta_p r^2} \, dv = \left(\frac{2\beta_p}{\pi}\right)^{3/2}$$

$$N_q^2 = \left\{ \int Z^2 \, e^{-2\beta_q r^2} \, dv \right\}^{-1} = 4\beta_q \left(\frac{2\beta_q}{\pi}\right)^{3/2}$$

$$T = \beta_p + \beta_q \; ; \qquad S = 4\pi \sin(\theta)/\lambda$$

1. $\langle S_L | S_L \rangle = N_p N_p \, e^{-i\bar{S}\cdot\bar{R}/2} \left(\frac{\pi}{T}\right)^{3/2} e^{-S^2/4T}$

2. $\langle S_L | S_R \rangle = N_p N_q \, e^{i\bar{S}\cdot\bar{R}/2(\beta_q-\beta_p)/T} \left(\frac{\pi}{T}\right)^{3/2} e^{-S^2/4T} \, e^{-R^2\beta_p\beta_q/T}$

q on right center

3. $$\langle P_L|P_L\rangle = N_qN_q\, e^{-\frac{i\bar{S}\cdot\bar{R}}{2} - S^2/4T}\left(\frac{\pi}{T}\right)^{3/2}\left\{\frac{1}{2T} - \frac{S_z^{\,2}}{4T^2}\right\}$$

4. $$\langle S_L|P_R\rangle = N_pN_q\, e^{i\bar{S}\cdot\bar{R}(\beta_p-\beta_q)/2T}\left(\frac{\pi}{T}\right)^{3/2} e^{-S^2/4T}\, e^{-R^2\beta_p\beta_q/T} \;.$$

$$\left\{\frac{iS_z-2R\beta_p}{2T}\right\}; \qquad q^{th} \text{ on right center}$$

5. $$\langle S_L|P_L\rangle = N_pN_q\, e^{-\frac{i\bar{S}\cdot\bar{R}}{2}}\left(\frac{\pi}{T}\right)^{3/2} e^{-S^2/4T}\,\frac{iS_z}{2T}\;; \quad q^{th} \text{ on left center}$$

6. $$\langle P_L|P_R\rangle = N_pN_q\, e^{-\frac{i\bar{S}\cdot\bar{R}}{2}}\, e^{-R^2\beta_p\beta_q/T}\left(\frac{\pi}{T}\right)^{3/2} e^{iS\cdot R\beta_q/T} \;.$$

$$\left\{\frac{1}{2T} + \frac{2i\bar{S}\cdot\bar{R}(\beta_q-\beta_p) - S_z^{\,2}-4R^2\beta_p\beta_q}{4T^2}\right\} \;; \quad q^{th} \text{ on right center}$$

Note that if subscripts denoting the centers are reversed in each of the equations above, the result is the respective complex conjugate.

Appendix B

Wavefunctions

1. Introduction

All systems studied in this work make use of Gaussian basis functions for the orbitals. These functions permit analytic formulations for the integrals and reasonable machine times for their evaluation.[42]

The central idea in this method is to expand Slater-type orbitals as a linear combination of Gaussian-type functions. The procedure then is to make these expansions approximate eigenfunctions of the Hamiltonian for which the Stater-type functions are exact eigenfunctions. This is the approach used by McWeeny[17] and Huzinaga.[42] Alternatively, the method of least squares may be applied to the Gaussian expansions and the exponents and expansion coefficients adjusted for a minimum error. This method was used by Boys and Shavitt[43] and Stewart.[44]

Both of the optimization processes are subject to pitfalls. The first, by the appearance of multiple minima[42] and the second because it emphasizes space-filling properties of the orbitals. Stewart[44] has shown the Gaussian orbitals to be satisfactory for studies of chemical properties and X-ray scattering factors.

2. Hydrogen

The wavefunctions used for the hydrogen-hydrogen interaction calculations are based on generalized valence bond orbitals, with spatial projection, rather than the traditional molecular orbitals. They were taken from a work performed by Huestis.[45]

The wavefunctions, consisting of Gaussian basis orbitals, are given by

$$\psi(r,R) = P\phi_1\phi_2\ \alpha\ \beta \tag{1}$$

where P is a symmetry and spin projection operator, and ϕ_1 and ϕ_2 are atomic orbitals. α,β are spin up and down respectively. The operator P, for the singlet state of hydrogen, has the form

$$P = (1+i)\Big[1 + \{12\}\Big]_{\text{space}} [1 - \{12\}]_{\text{spin}} \tag{2}$$

The many-electron wavefunction, at a given separation R, is

$$\psi(r,R) = [\phi_{1L}\ \phi_{2R}+\ \phi_{2R}\phi_{1L}+\phi_{1R}\phi_{2L}+\phi_{2L}\phi_{1R}]\ [\alpha\beta-\beta\alpha] \tag{3}$$

where the position of ϕ_{iR},ϕ_{iL} indicates the atomic orbital to which it pertains. The subscript L or R indicates an orbital whose main contribution is to be found on the left (L) or right (R) center. Thus, in the expression for charge density, a term of the form $\phi_{1L}\phi_{1L}^*$ and $\phi_{1R}\phi_{1R}^*$ represent a distribution centered mainly on L or R respectively. For large separations, these two terms represent the density distributions of two isolated atoms.

The orbitals ϕ_{iL} and ϕ_{jR} are given by an expansion of contracted basis functions χ_μ,

$$\phi_i = \sum_\mu C_i^\mu\ \chi_\mu \tag{4}$$

where the C_i^μ are orbital coefficients and χ_μ is given by the expansion

$$\chi_\mu = \sum_\alpha B_\mu^\alpha \theta_\alpha \qquad (5)$$

B_μ^α is the contraction coefficient and θ_α are the normalized primitive Gaussian basis functions of the type

$$\theta_\alpha = N_\alpha e^{-\beta_\alpha r^2} \qquad (6)$$

or

$$\theta_\alpha = N_\alpha z\ e^{-\beta_\alpha r^2} \qquad (7)$$

N_α is the normalization constant.

3. Helium

The molecular orbitals for helium were taken from work done by Ransil.[46]

The ground state of a helium molecule is described by the wavefunction

$$\psi(r,R) = \sigma_g(r,R)\ \sigma_\mu(r,R)\,[\alpha\beta-\beta\alpha] \qquad (1)$$

where α,β are the usual spin functions and σ_g,σ_μ are the spatial orbitals. Each of the spatial orbital types is formed by a linear combination of atomic orbitals centered on L and R. Thus, for the sigma-g type,

$$\sigma_g = C_{11}1S_L + C_{12}2S_L + C_{13}2P_L + C_{14}1S_R + C_{15}2S_R + C_{16}2P_R \qquad (2)$$

The Slater orbitals of eq. (2) are further expressed as Gaussian expansions, given by Huzinaga.[42] Denoting a Slater orbital by ψ_s, then

$$\psi_s = \sum_i C_i \chi_{g,i} \tag{3}$$

where $\chi_{g,i}$ is a normalized Gaussian orbital of the form

$$\chi_{g,i} = r^{n_g-1} \exp(-\rho_g r)\ Y_{\ell m}(\theta,\phi) \tag{4}$$

and C_i are expansion coefficients that normalize ψ_s. The Slater orbitals have the form

$$\psi_s = r^{n_s-1} \exp(-\rho_s r)\ Y_{\ell m}(\theta,\phi) \tag{5}$$

and

$$\rho_{g,i} = (n_s \rho_s)^2 \alpha_i$$

4. Argon

The molecular orbitals for argon were taken from work performed by Gilbert and Wahl.[47] These orbitals are given by the expansion

$$\psi_{i,\alpha} = \sum_\rho C_{i\lambda\rho} \omega_{\rho,\alpha} \tag{1}$$

of unnormalized basis functions,

$$\omega_{\rho,\alpha} = [\chi_{plm}(\bar{r}-\bar{R}_L) \pm (-1)^\ell \chi_{plm}(\bar{r}-\bar{R}_R)]/\sqrt{2} \tag{2}$$

where the $\chi_{plm}(\bar{r})$ are normalized atomic basis functions,

$$\chi_{plm}(\bar{r}) = [2n_{p\ell}!]^{-\frac{1}{2}}(2\rho_{p\ell})^{n_{p\ell}+\frac{1}{2}}\; r^{n_{p1}-1}\; \exp(-\rho_{p\ell}r)Y_{\ell m}(\theta,\phi) \qquad (3)$$

The indices ρ, λ, α are the principal, symmetry, and partner indices for molecular basis functions. p,ℓ,m are the corresponding indices for atomic basis functions. The coefficients $C_{i\lambda\rho}$ are obtained by solving the Hartree-Fock equations. The coefficients and exponents for the expansion of the Slater orbitals in terms of Gaussians are the same as used for the helium wavefunction.

Appendix C

Figures 1 - 42

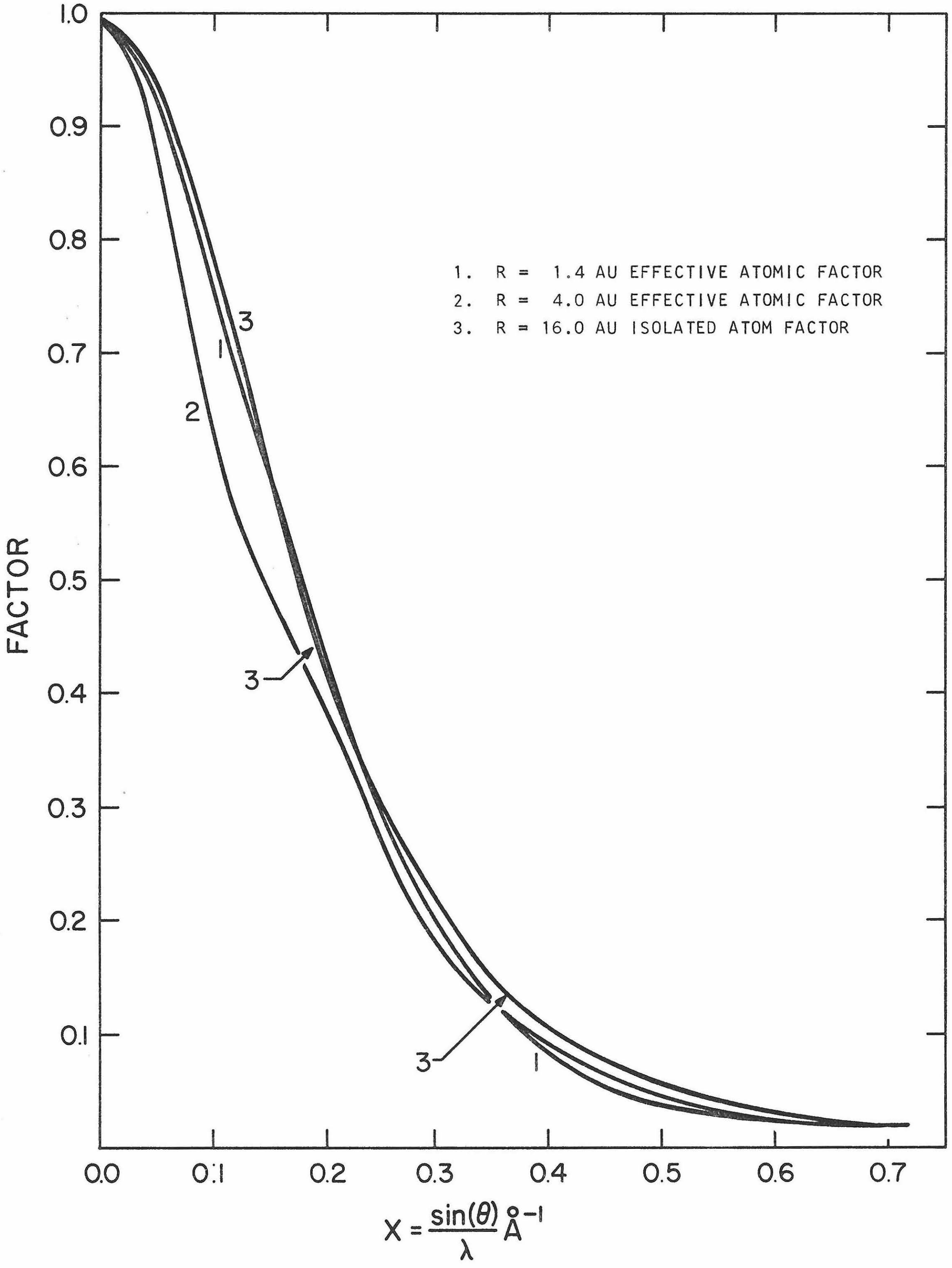

FIGURE 1. MAGNITUDE OF THE EFFECTIVE FACTORS F_P (R, S) AND ISOLATED ATOM FACTOR F_P (∞, S). ORIENTATION = 0.0 RAD. SINGLET STATE OF HYDROGEN.

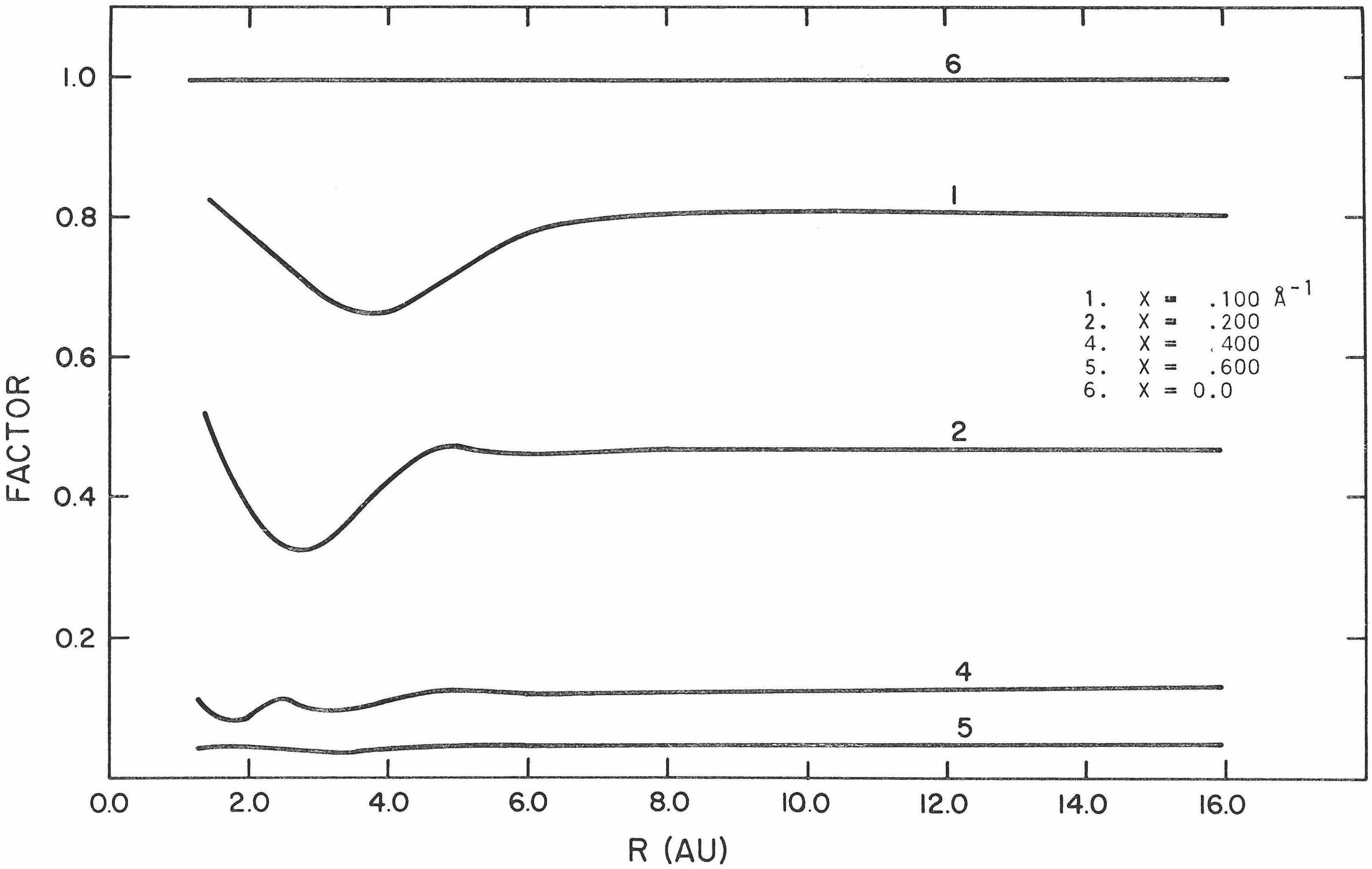

FIGURE 2 MAGNITUDE OF EFFECTIVE FACTOR FOR SELECT VALUES OF X. SINGLET STATE OF HYDROGEN. ORIENTATION = 0.0 RAD.

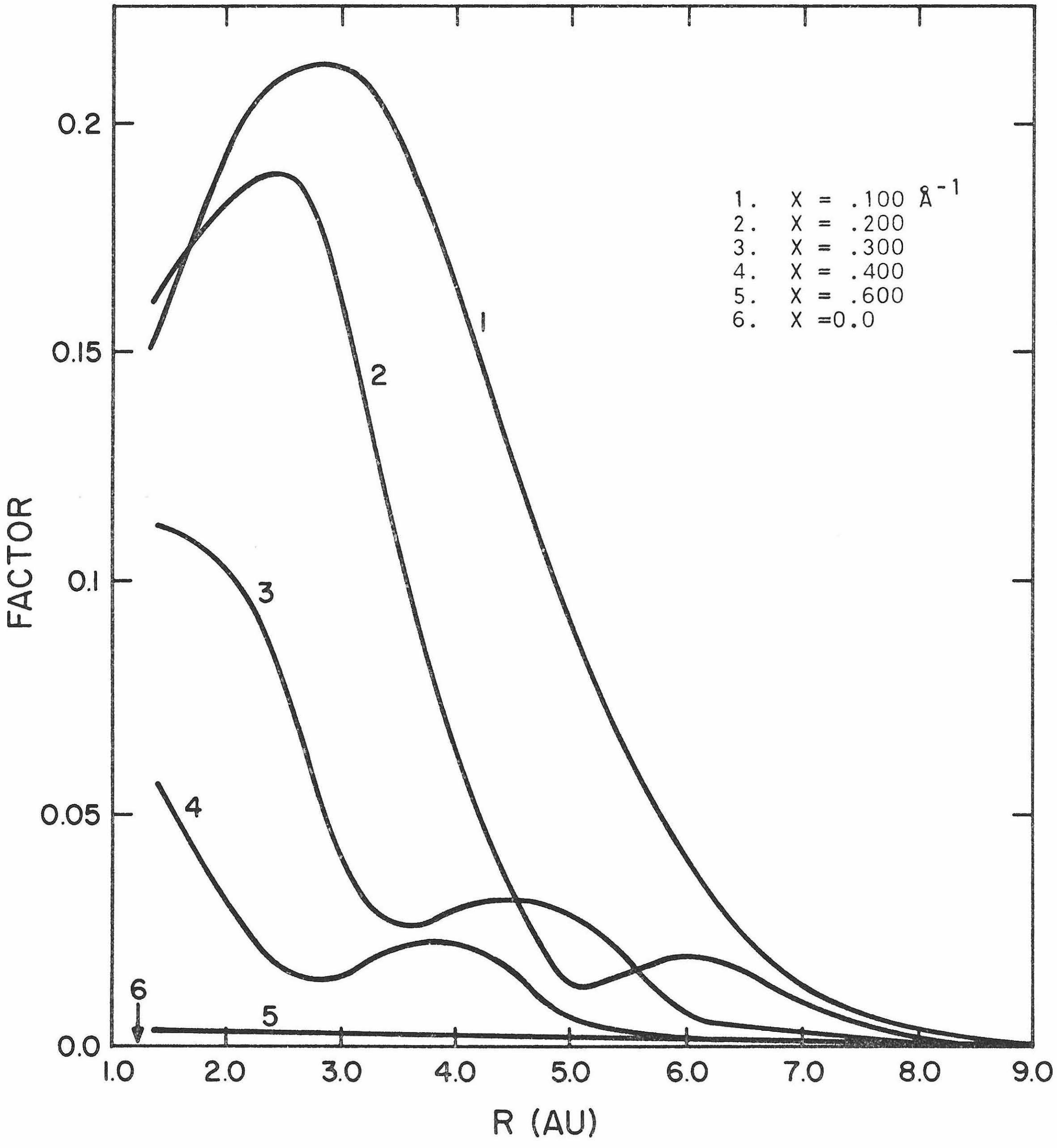

FIGURE 3. MAGNITUDE OF CORRECTION TO BE APPLIED TO THE ISOLATED ATOM FACTOR. ORIENTATION = 0.0 RAD. SINGLET STATE OF HYDROGEN.

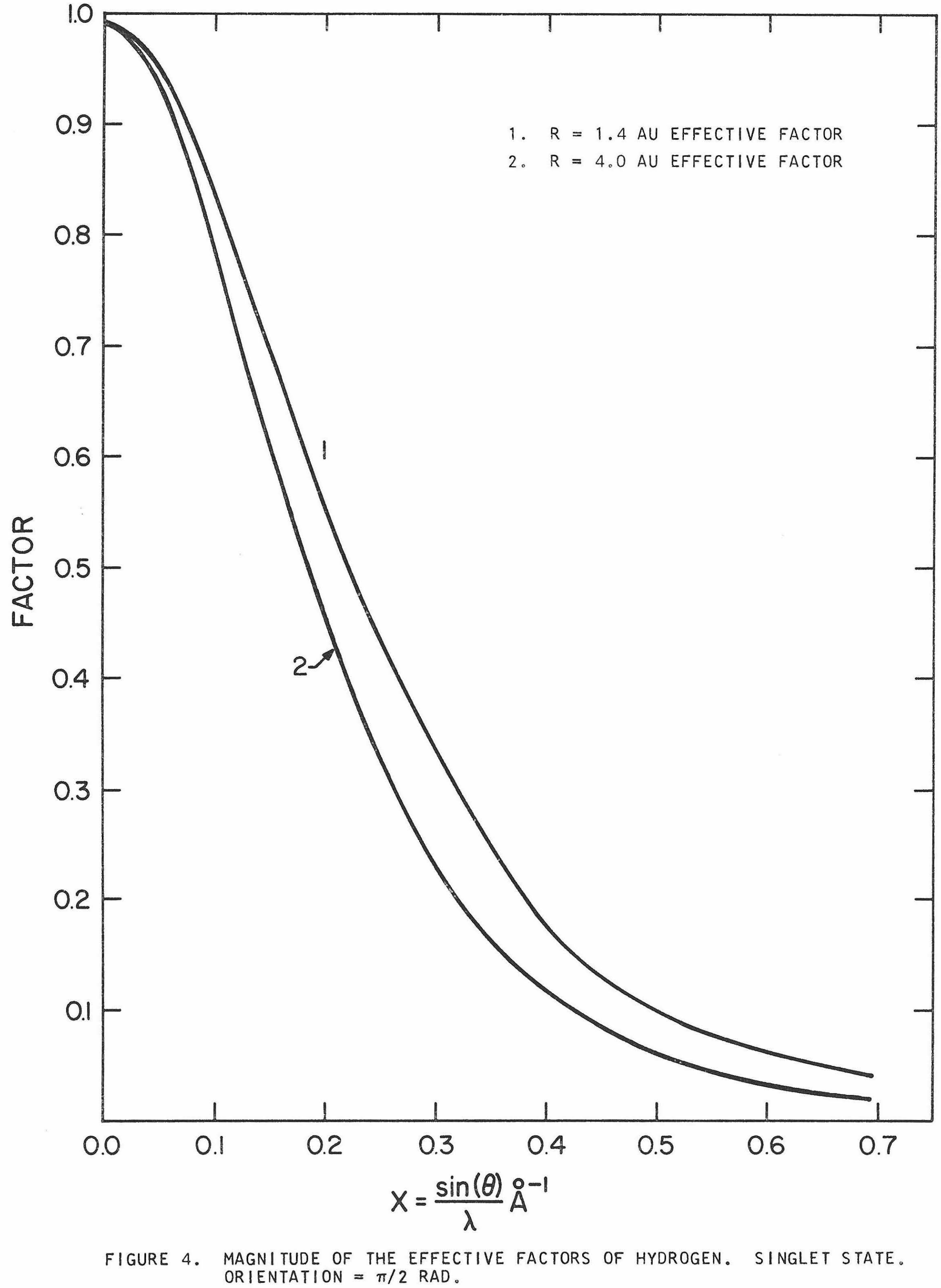

FIGURE 4. MAGNITUDE OF THE EFFECTIVE FACTORS OF HYDROGEN. SINGLET STATE. ORIENTATION = $\pi/2$ RAD.

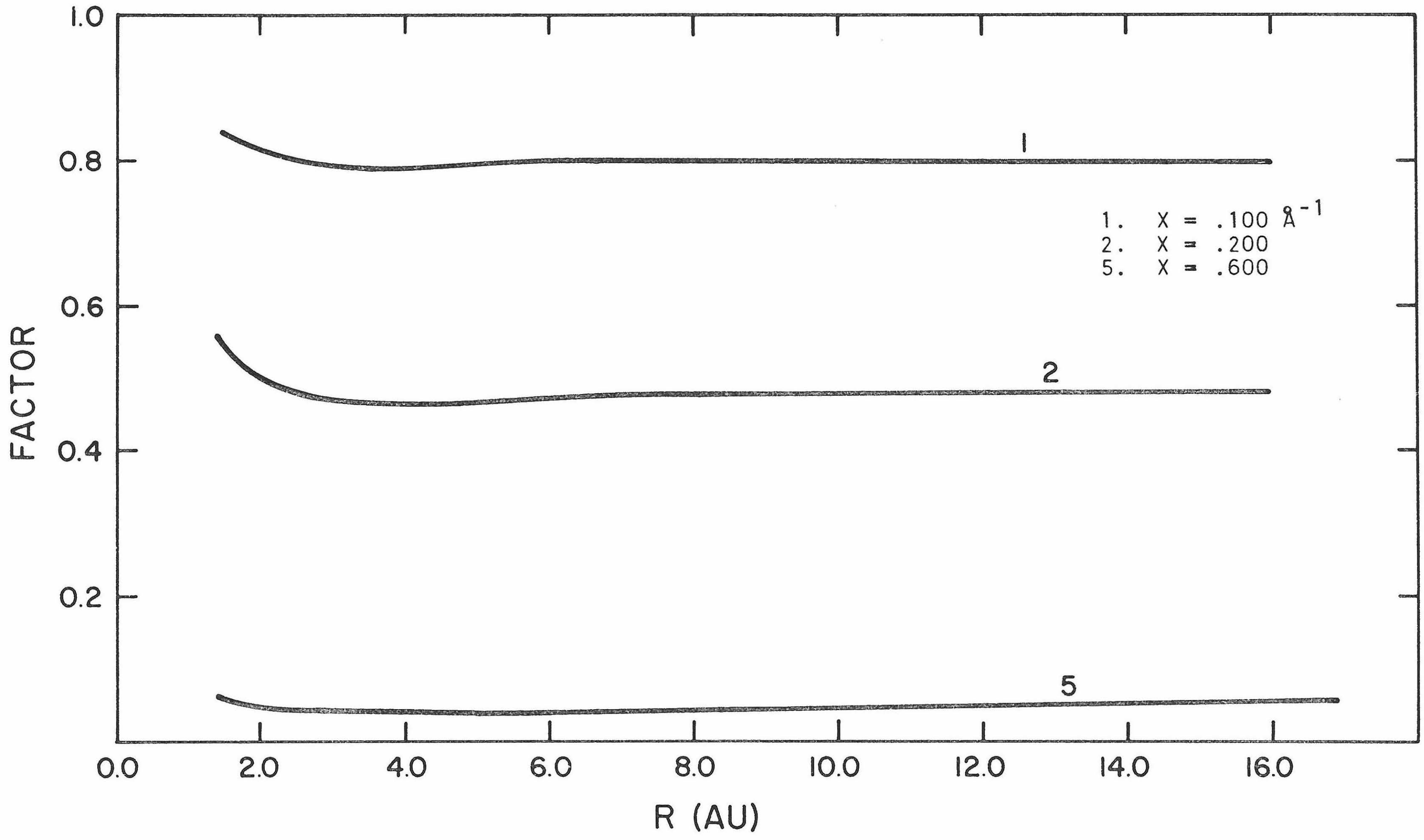

FIGURE 5. MAGNITUDE OF THE EFFECTIVE FACTOR FOR SELECT VALUES OF X. SINGLET STATE OF HYDROGEN. ORIENTATION = $\pi/2$ RAD.

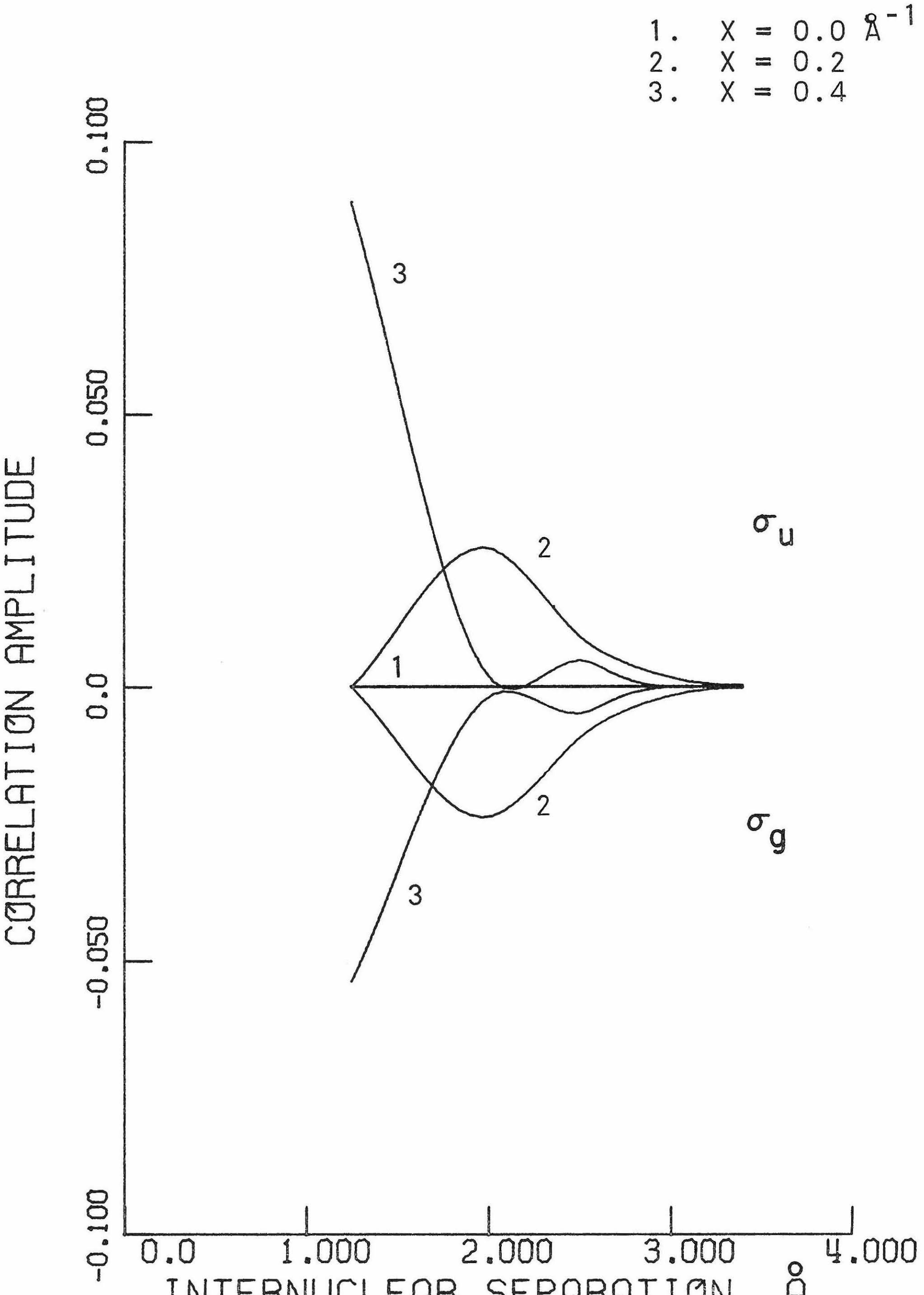

FIG. 6. REAL CORRELATION AMPLITUDES FOR HE. COMPARISON OF SIGMA-G AND SIGMA-U ORBITALS. ORIENTATION ANGLE=0.0

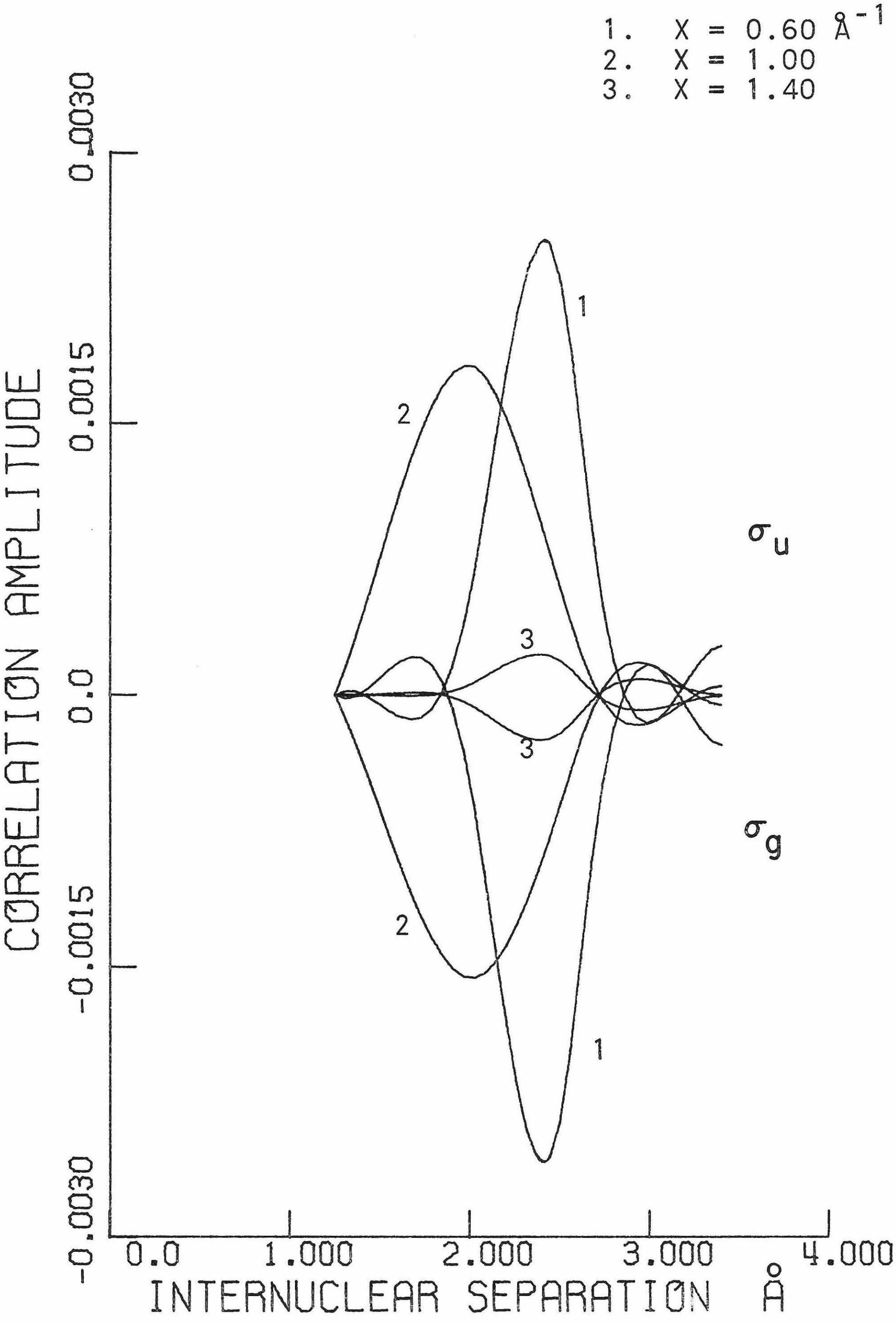

FIG. 7. REAL CORRELATION AMPLITUDES FOR HE. COMPARISON OF SIGMA-G AND SIGMA-U ORBITALS. ORIENTATION ANGLE=0.0

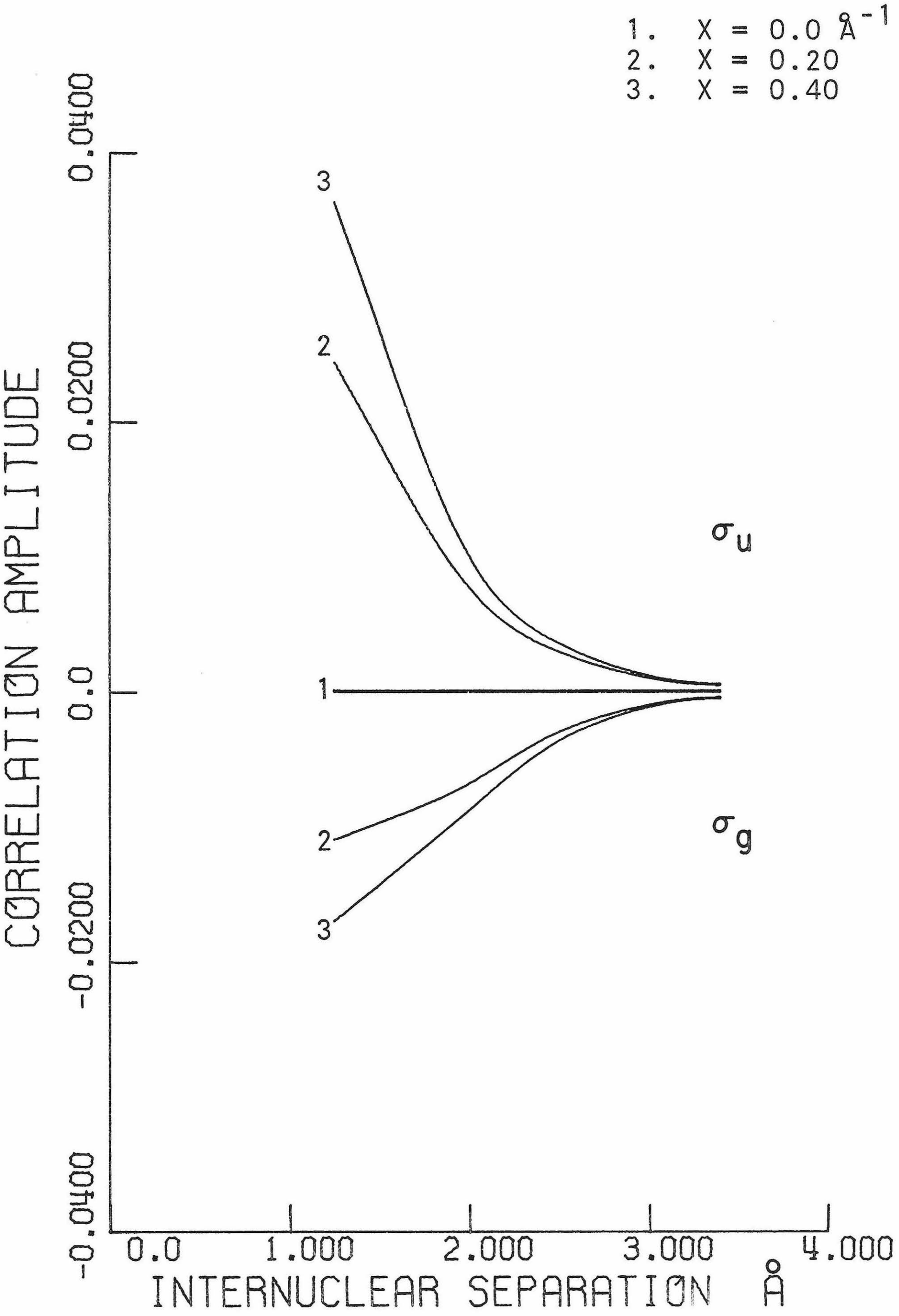

FIG. 8. REAL CORRELATION AMPLITUDES FOR HE.
COMPARISON OF SIGMA-G AND SIGMA-U ORBITALS.
ORIENTATION ANGLE=1.5708

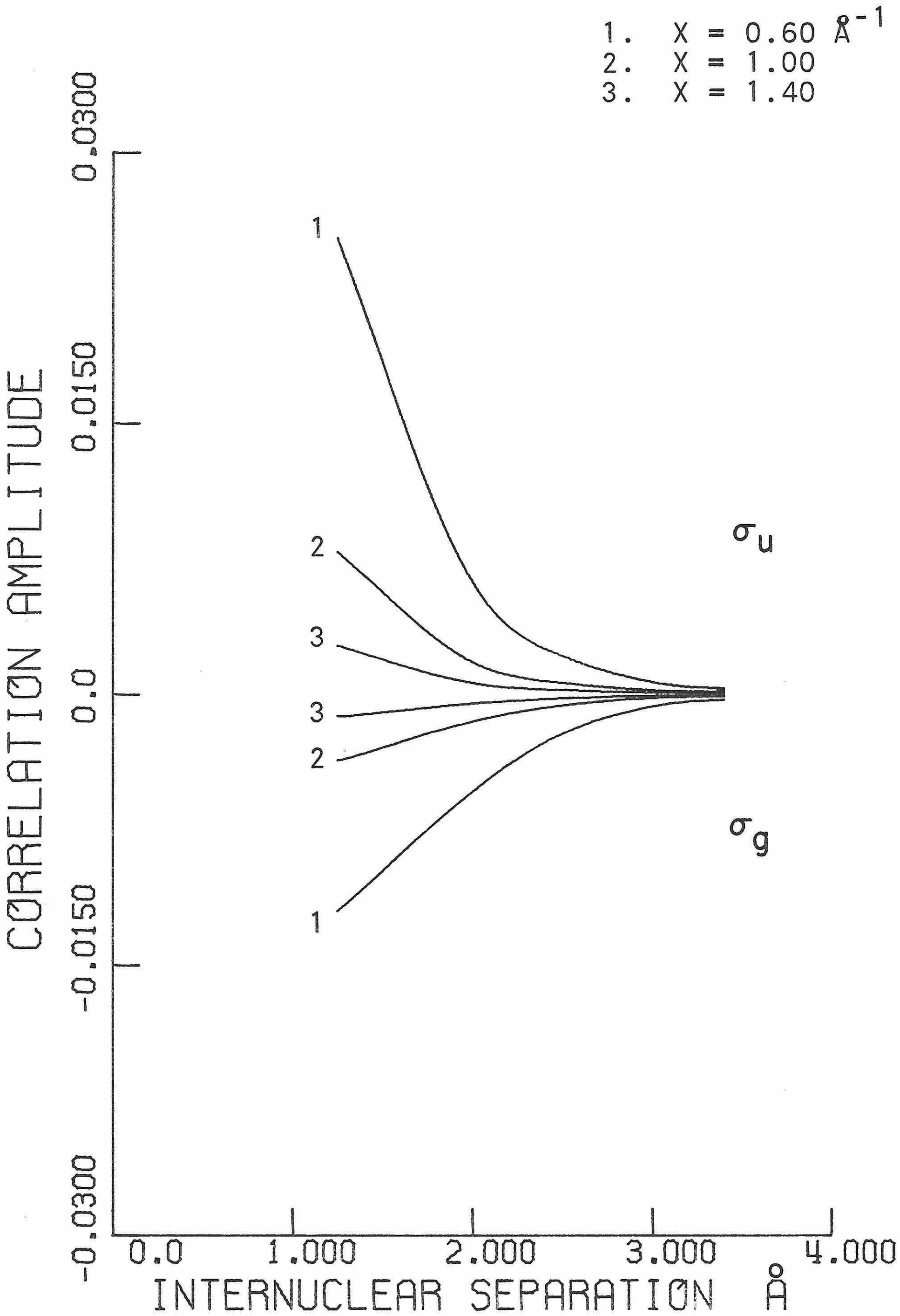

FIG. 9. REAL CORRELATION AMPLITUDES FOR HE.
COMPARISON OF SIGMA-G AND SIGMA-U ORBITALS.
ORIENTATION ANGLE=1.5708

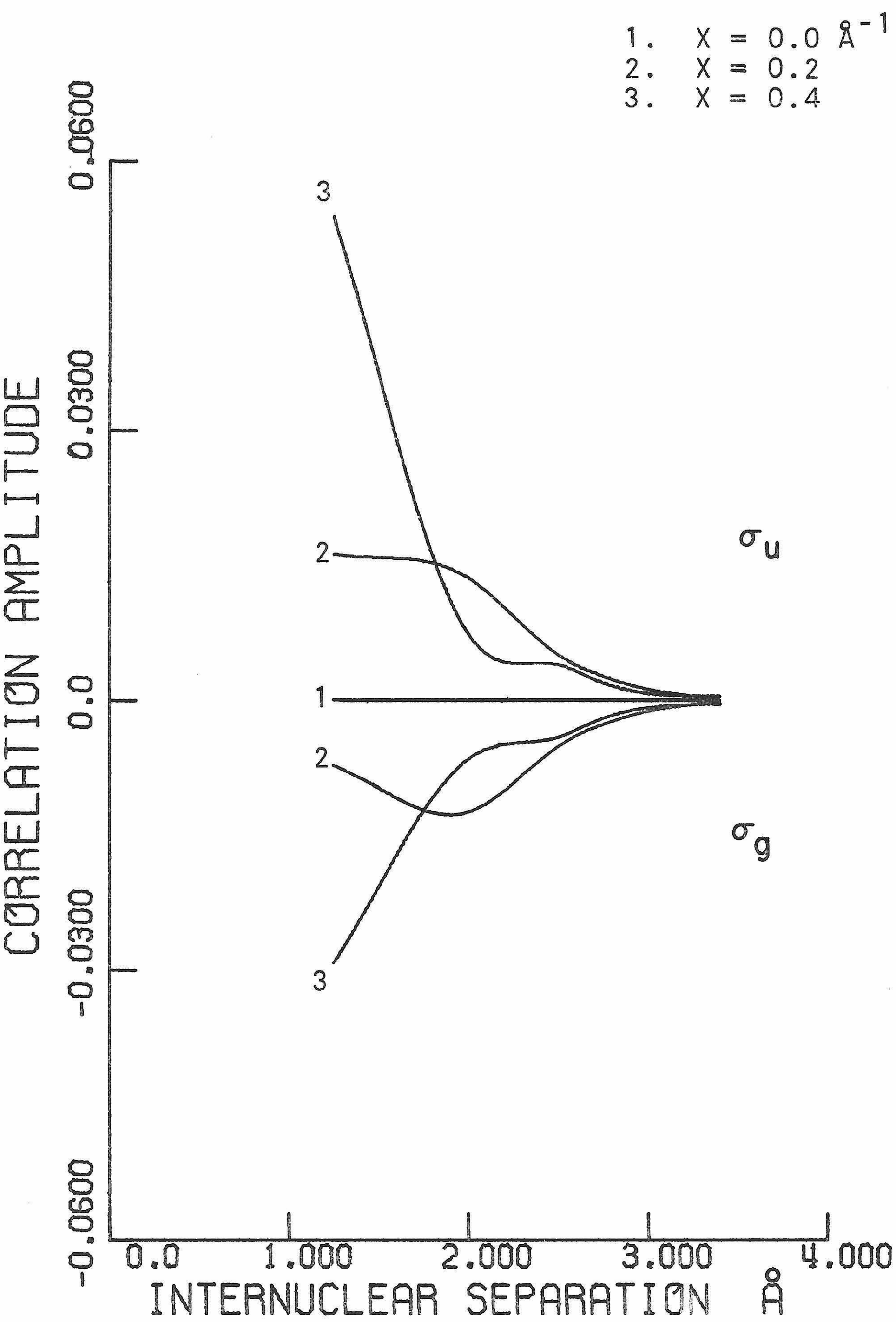

FIG. 10. COMPARISON OF ORIENTATIONALLY AVERAGED CORRELATION AMPLITUDES FOR HE SIGMA-G AND SIGMA-U ORBITALS

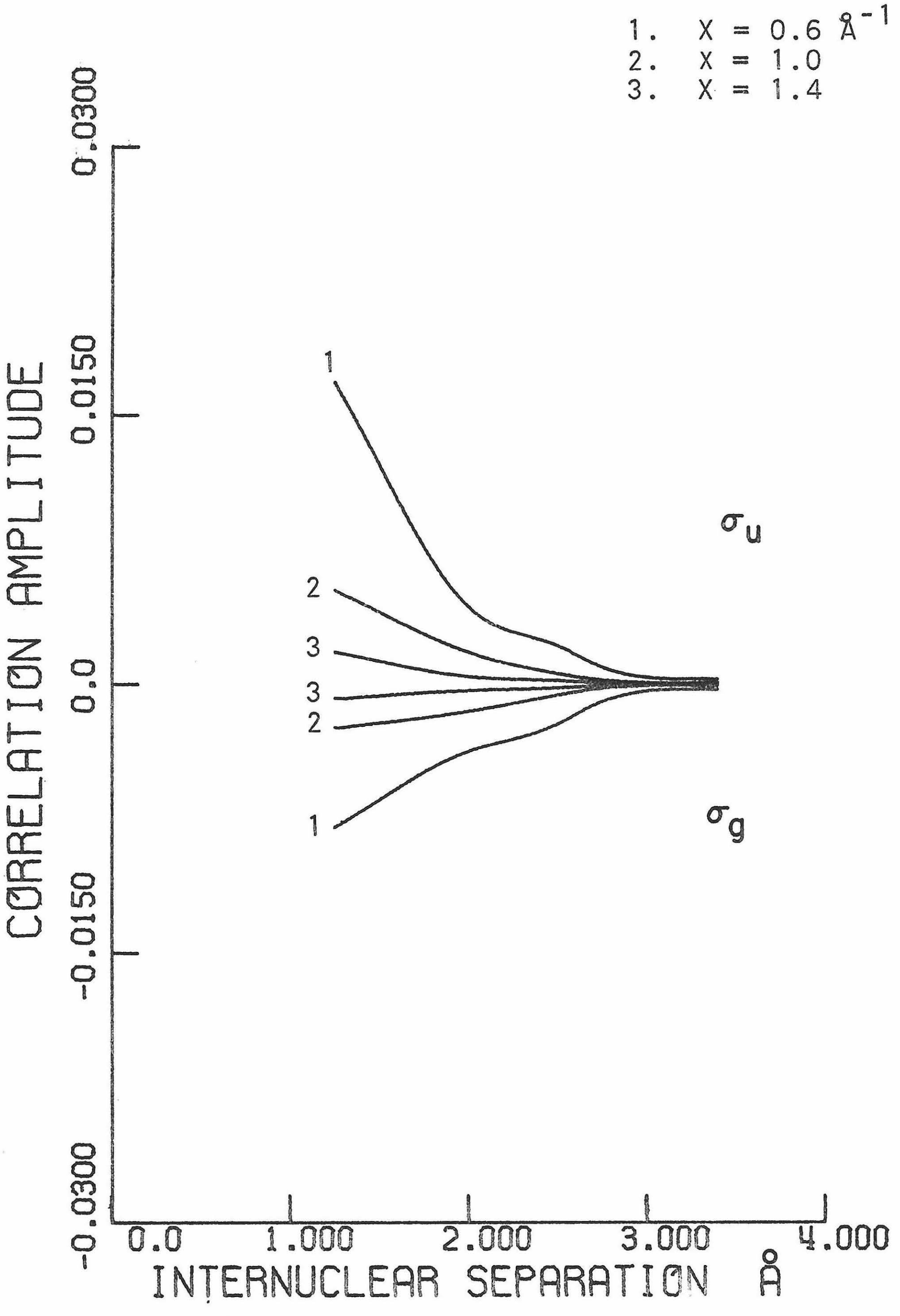

FIG. 11. COMPARISON OF ORIENTATIONALLY AVERAGED CORRELATION AMPLITUDES FOR HE SIGMA-G AND SIGMA-U ORBITALS

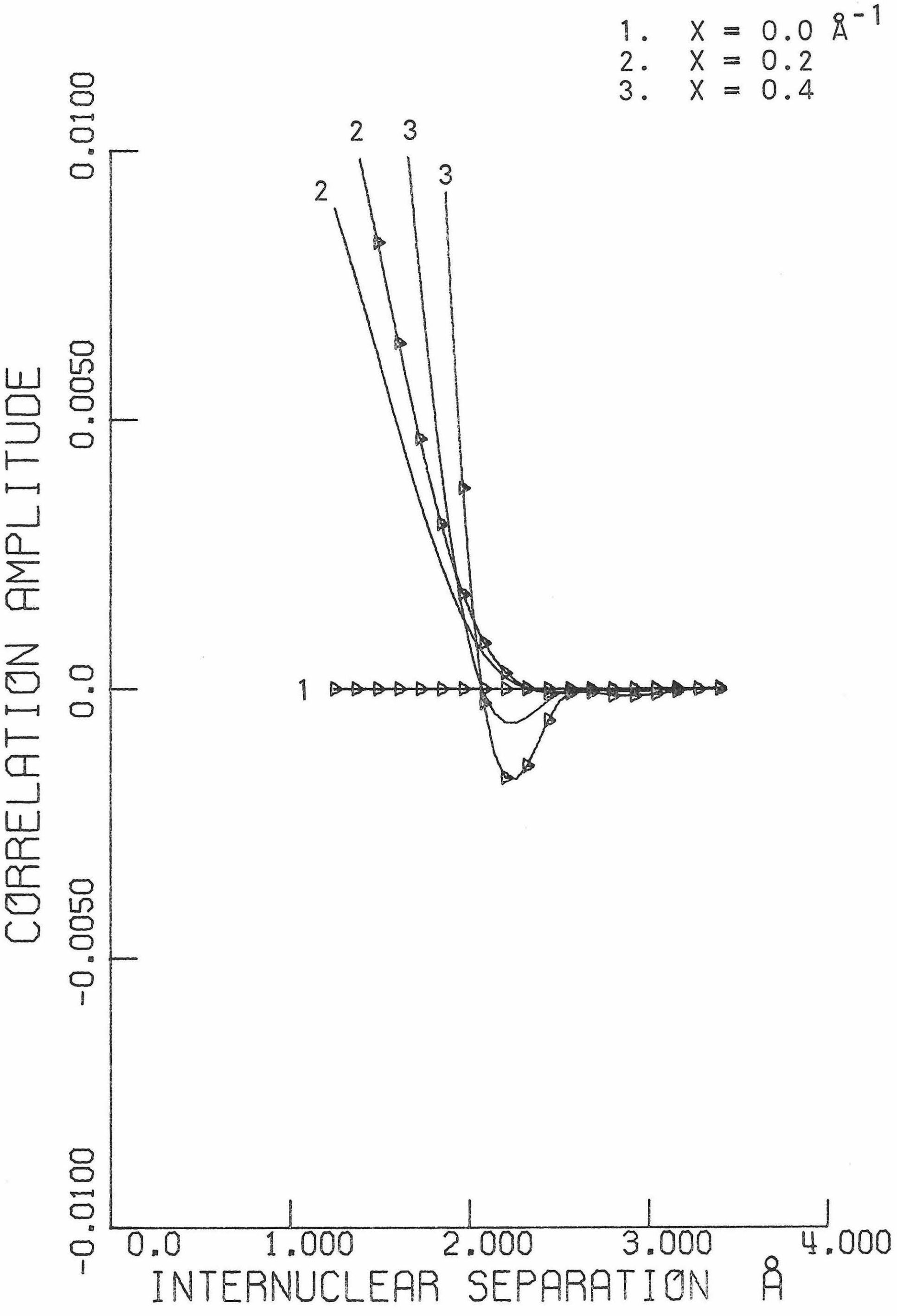

FIG. 12. COMPARISON OF ——— NET CORRELATION AMPLITUDES ORIENTATIONAL AVERAGE △△△ RATIO OF NET CORRELATION TO ISOLATED HE ATOM AMPLITUDE

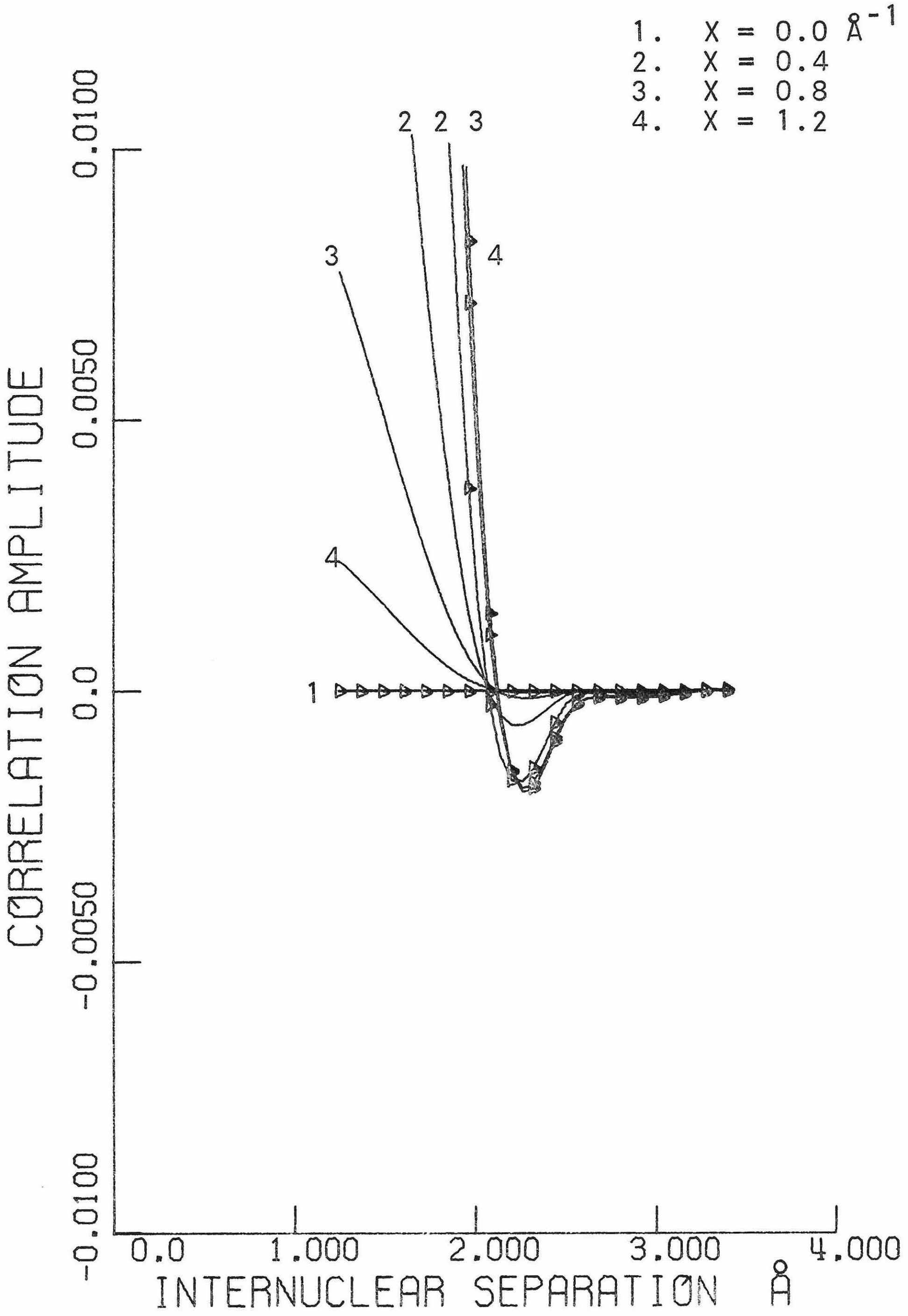

FIG. 13. COMPARISON OF —— NET CORRELATION AMPLITUDES ORIENTATIONAL AVERAGE -△△△- RATIO OF NET CORRELATION TO ISOLATED HE ATOM AMPLITUDE

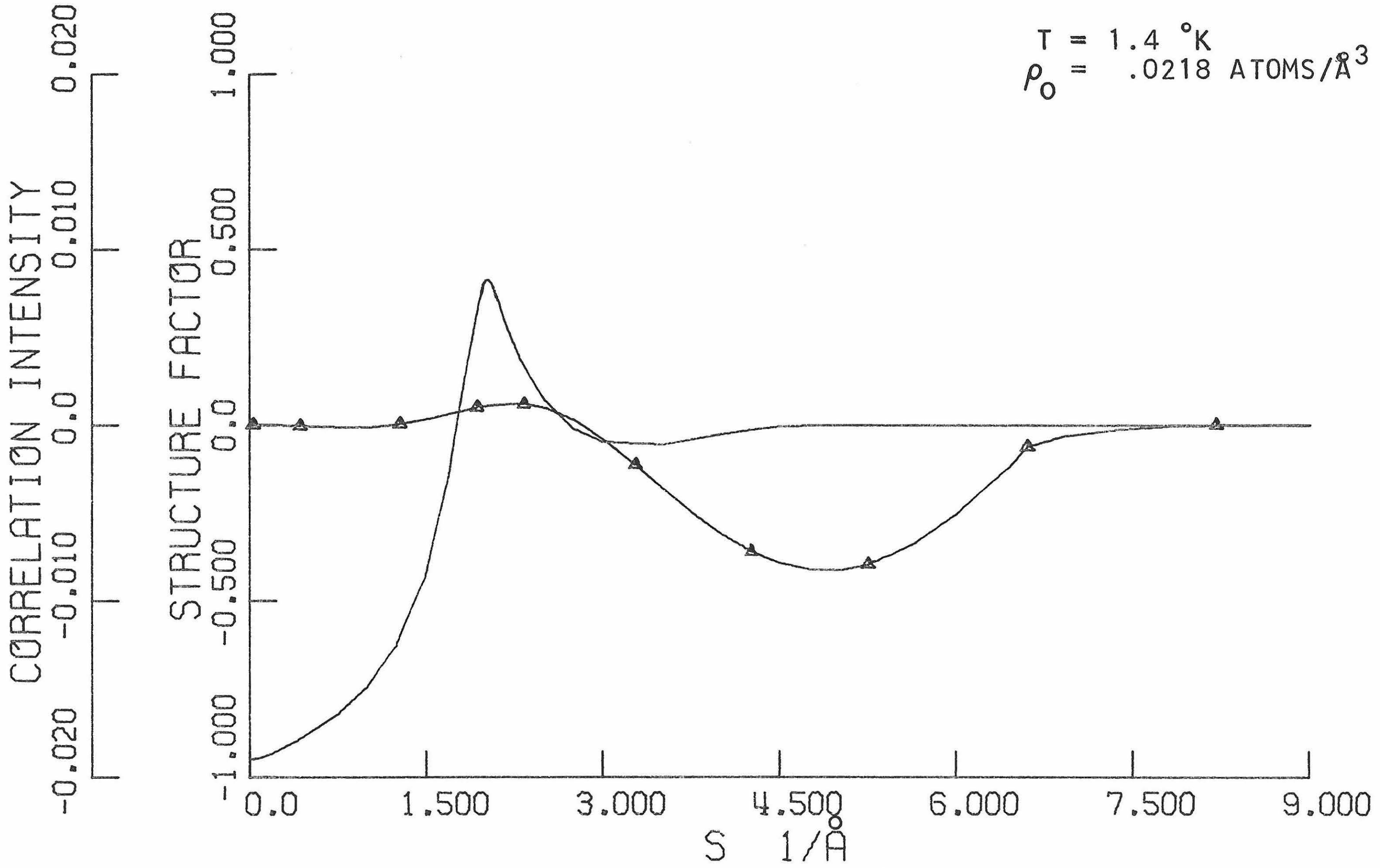

FIG. 14. —— STRUCTURE FACTOR FROM HE X-RAY DATA
ΔΔΔ CORRECTION DUE TO CORRELATION

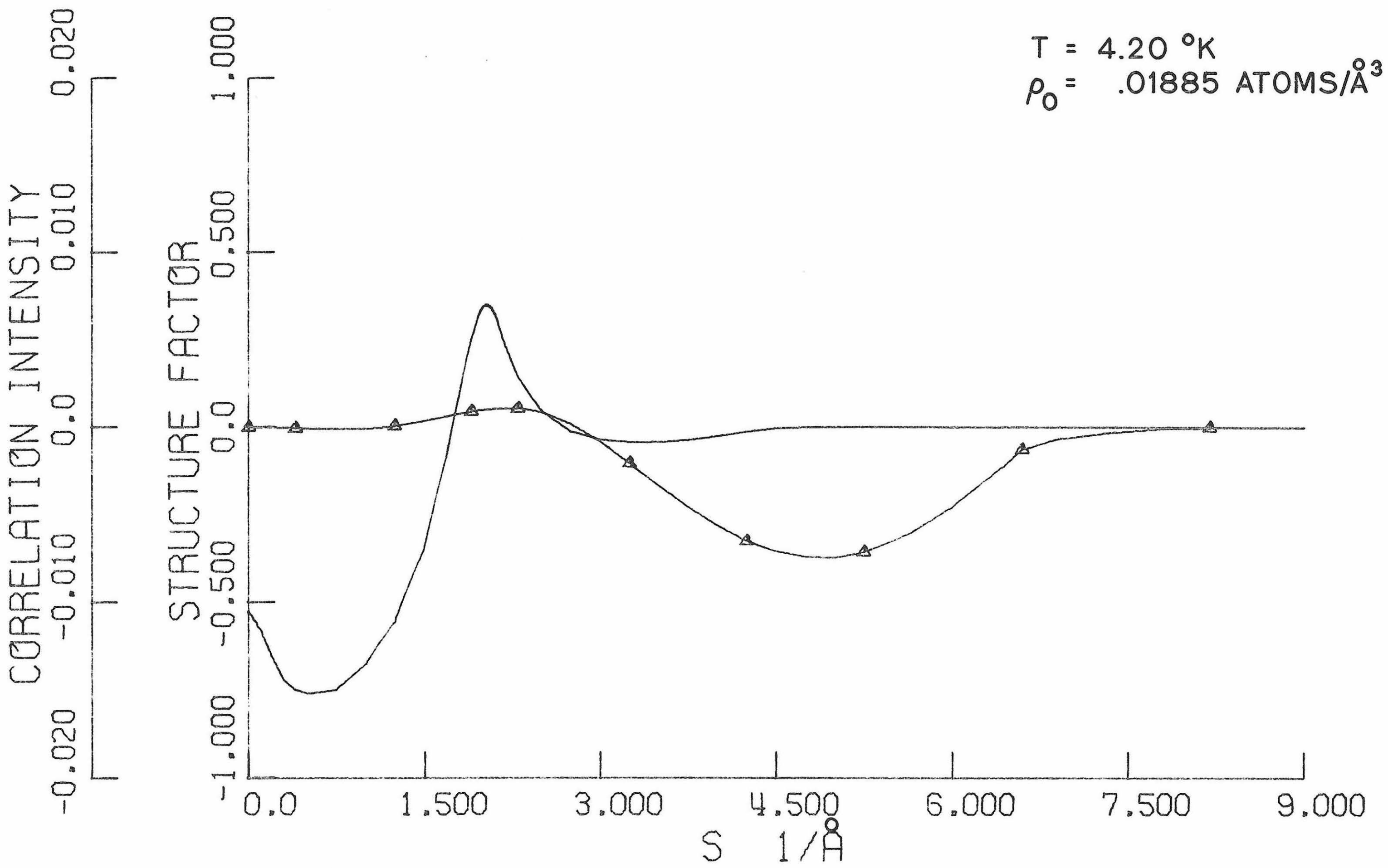

FIG. 15. —— STRUCTURE FACTOR FROM HE X-RAY DATA
△△△ CORRECTION DUE TO CORRELATION

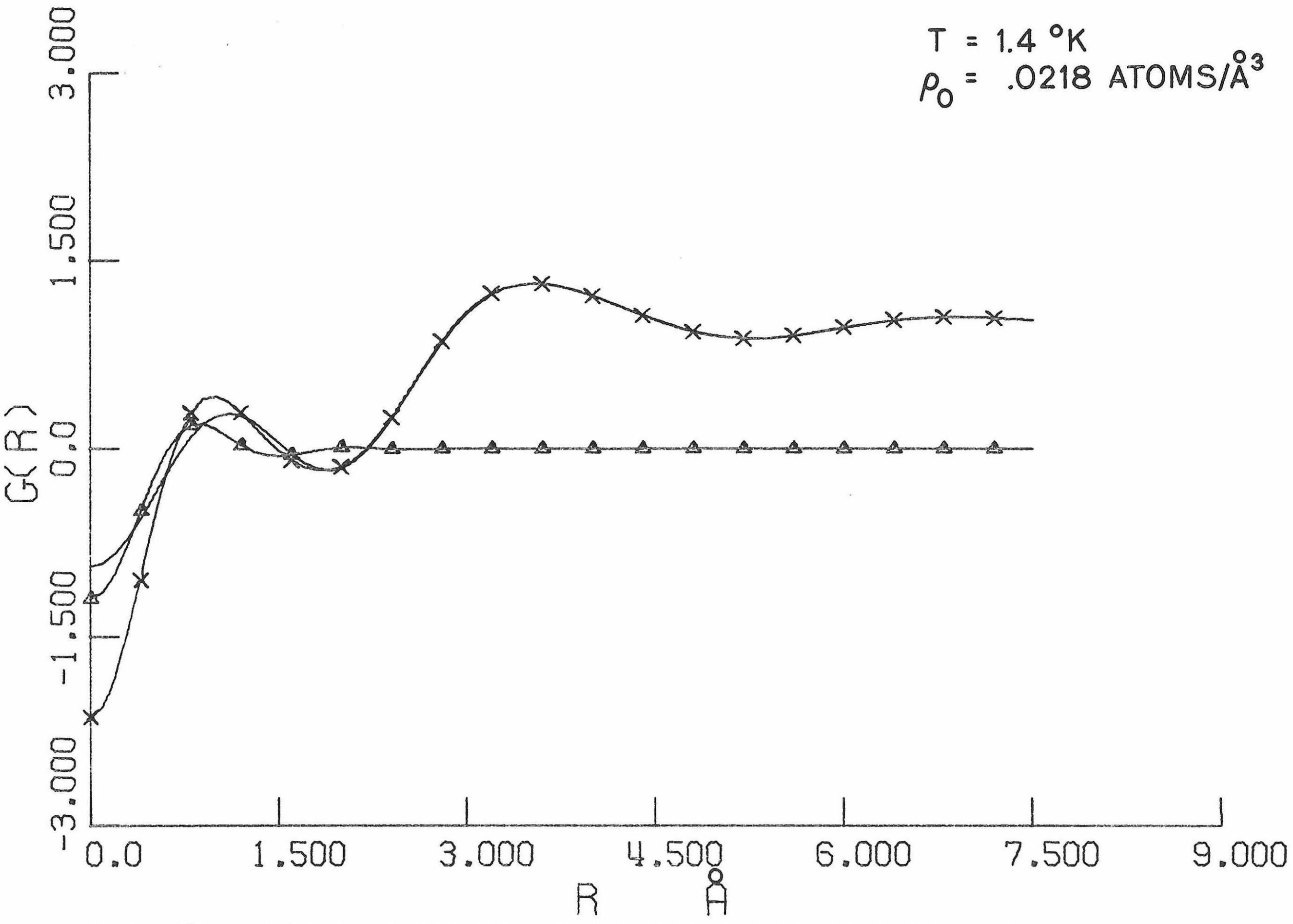

FIG. 16. RADIAL DISTRIBUTION FUNCTIONS FROM HE X-RAY DATA.
—— UNCORRELATED SCATTERING ‑×‑×‑× CORRELATED SCATTERING
‑△‑△‑△ DEVIATION DUE TO CORRELATION

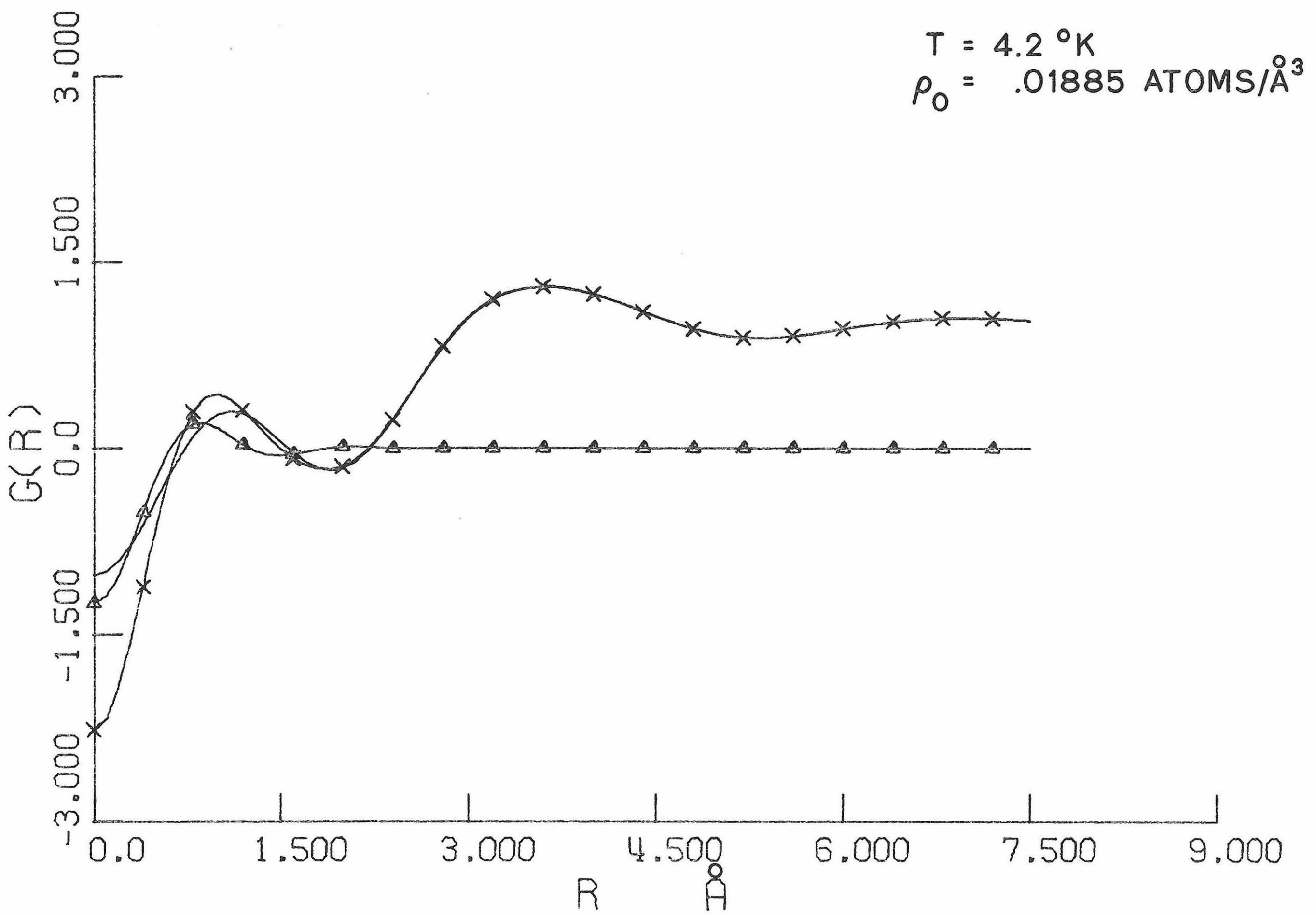

FIG. 17. RADIAL DISTRIBUTION FUNCTIONS FROM HE X-RAY DATA.
—— UNCORRELATED SCATTERING ✕✕✕ CORRELATED SCATTERING
△△△ DEVIATION DUE TO CORRELATION

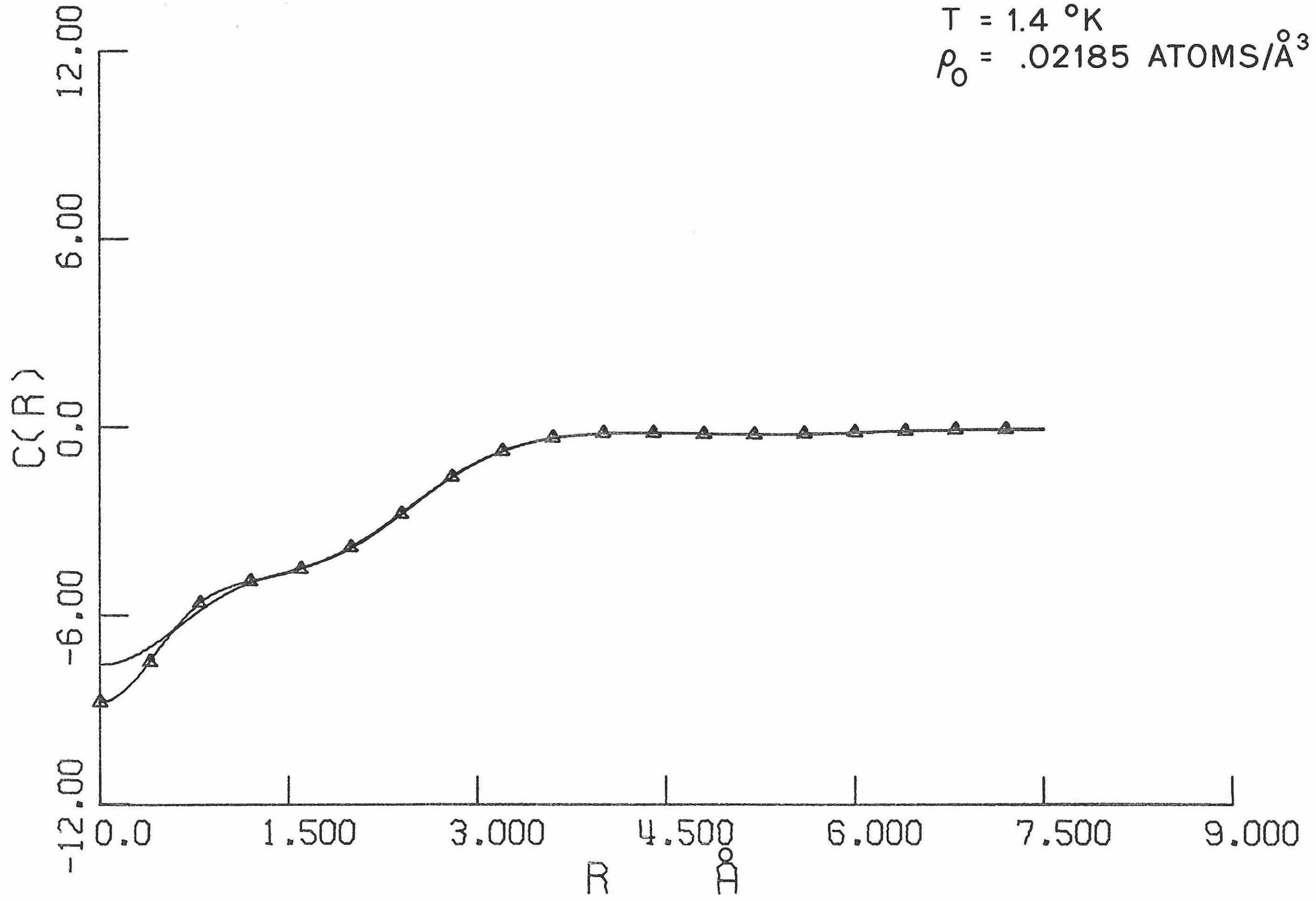

FIG. 18. DIRECT CORRELATION FUNCTIONS FROM HE X-RAY DATA.
—— UNCORRELATED SCATTERING -△-△-△- CORRELATED SCATTERING

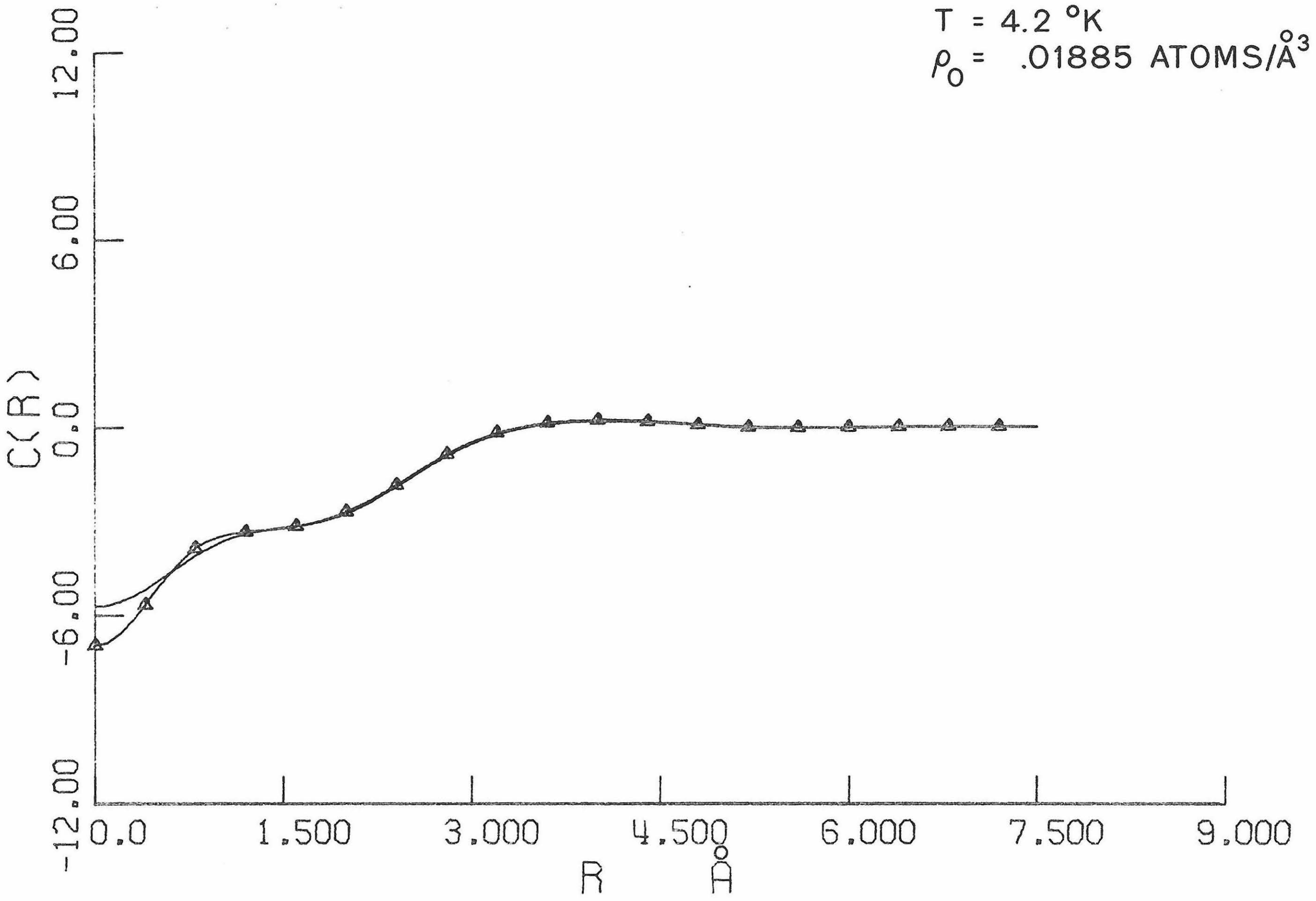

FIG. 19. DIRECT CORRELATION FUNCTIONS FROM HE X-RAY DATA.
——— UNCORRELATED SCATTERING -△-△-△- CORRELATED SCATTERING

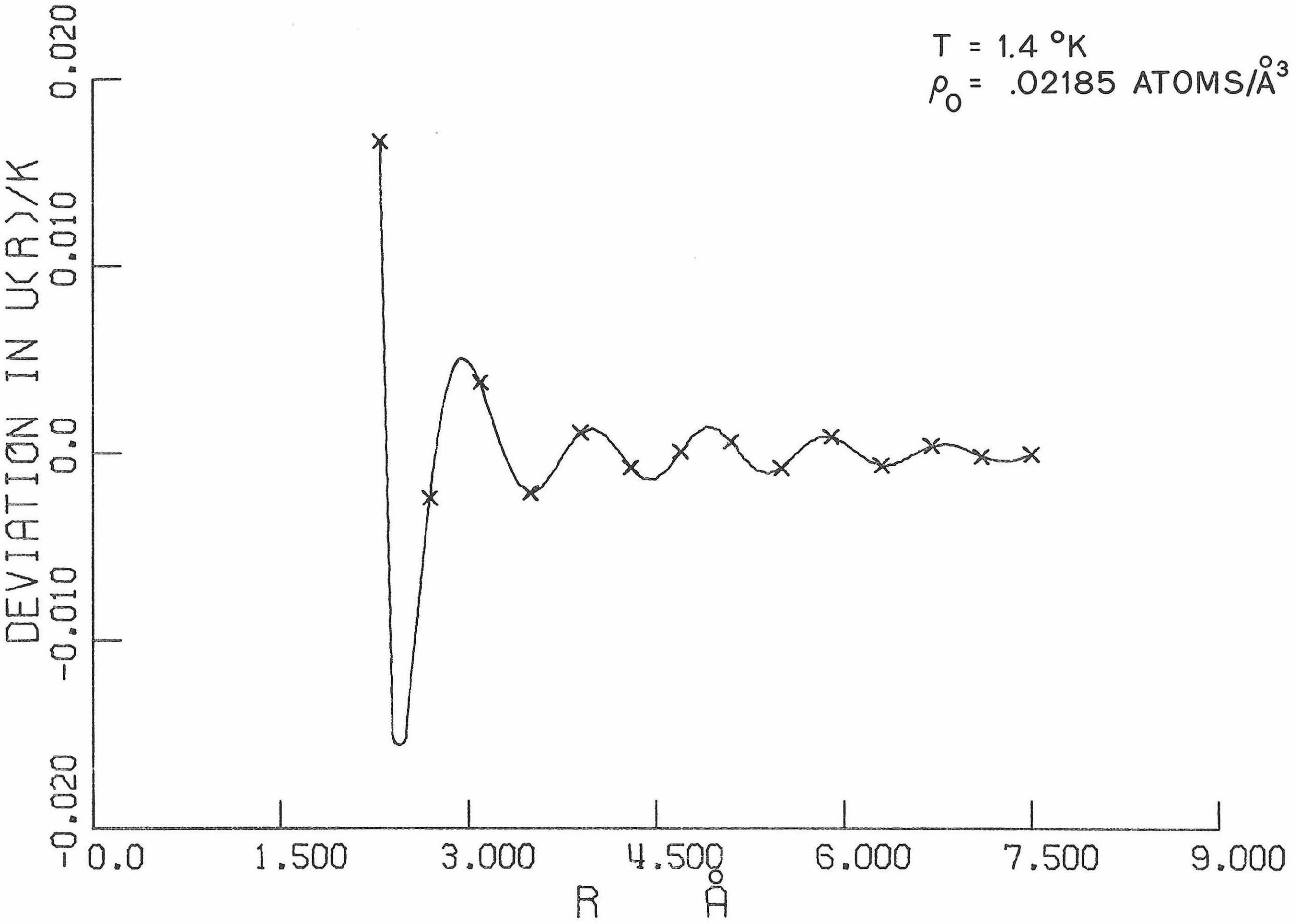

FIG. 20. POTENTIAL ENERGY DIFFERENCE FOR HELIUM, HNC THEORY
U(CORRELATED)/K − U(UNCORRELATED)/K

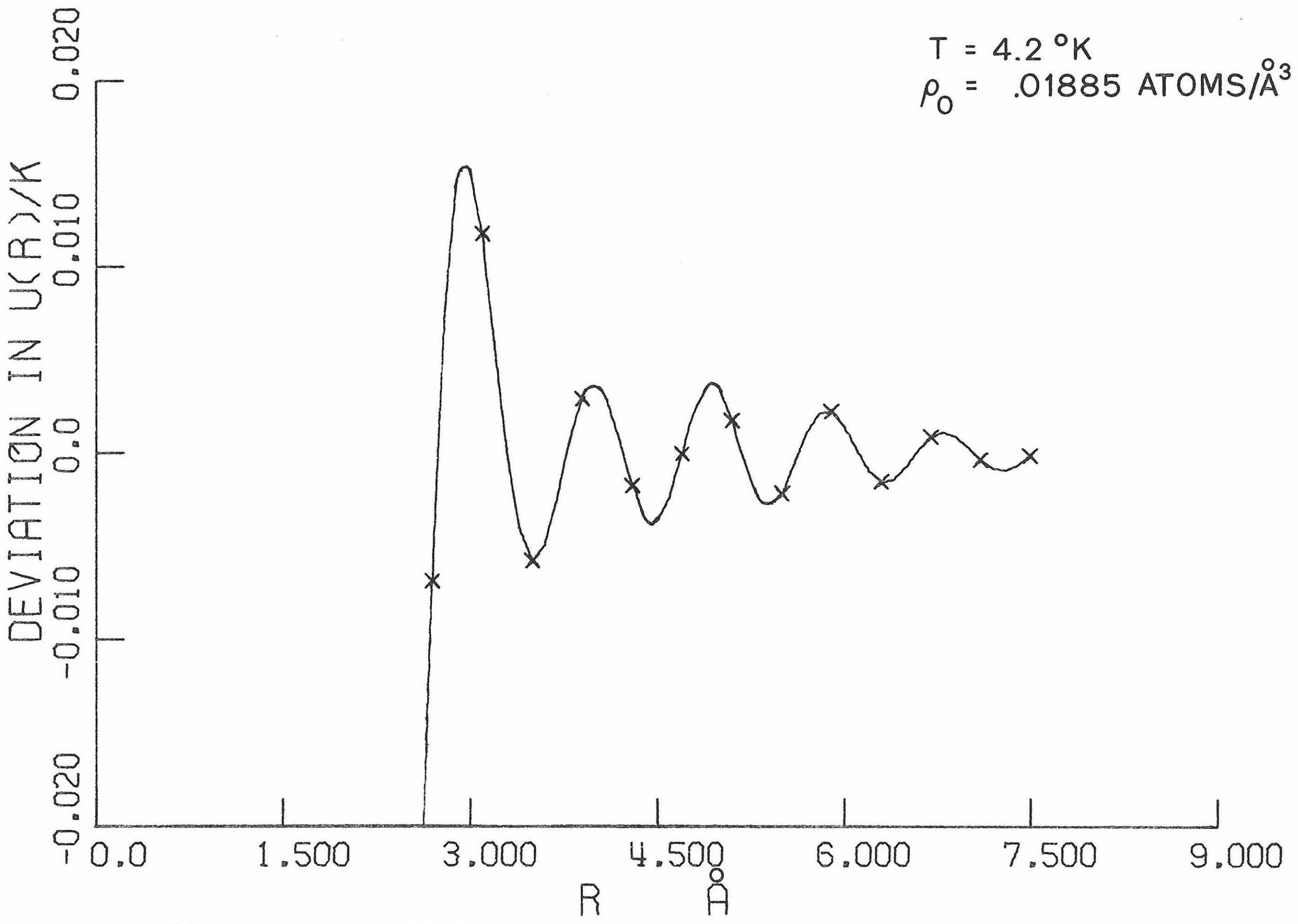

FIG. 21. POTENTIAL ENERGY DIFFERENCE FOR HELIUM, HNC THEORY
U(CORRELATED)/K − U(UNCORRELATED)/K

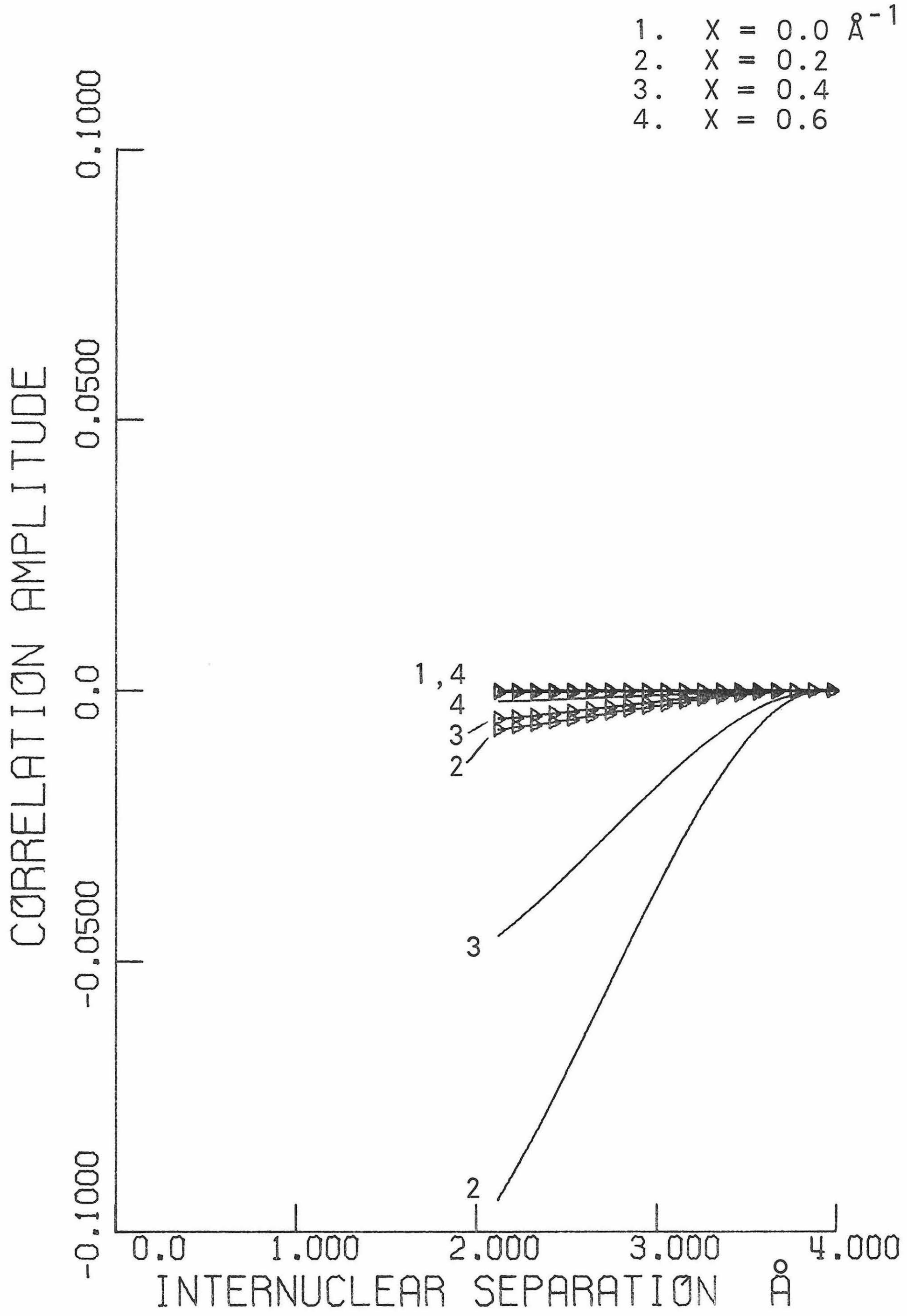

FIG. 22. COMPARISON OF ——— NET CORRELATION AMPLITUDES ORIENTATIONAL AVERAGE -△-△-△- RATIO OF NET CORRELATION TO ISOLATED AR ATOM AMPLITUDE

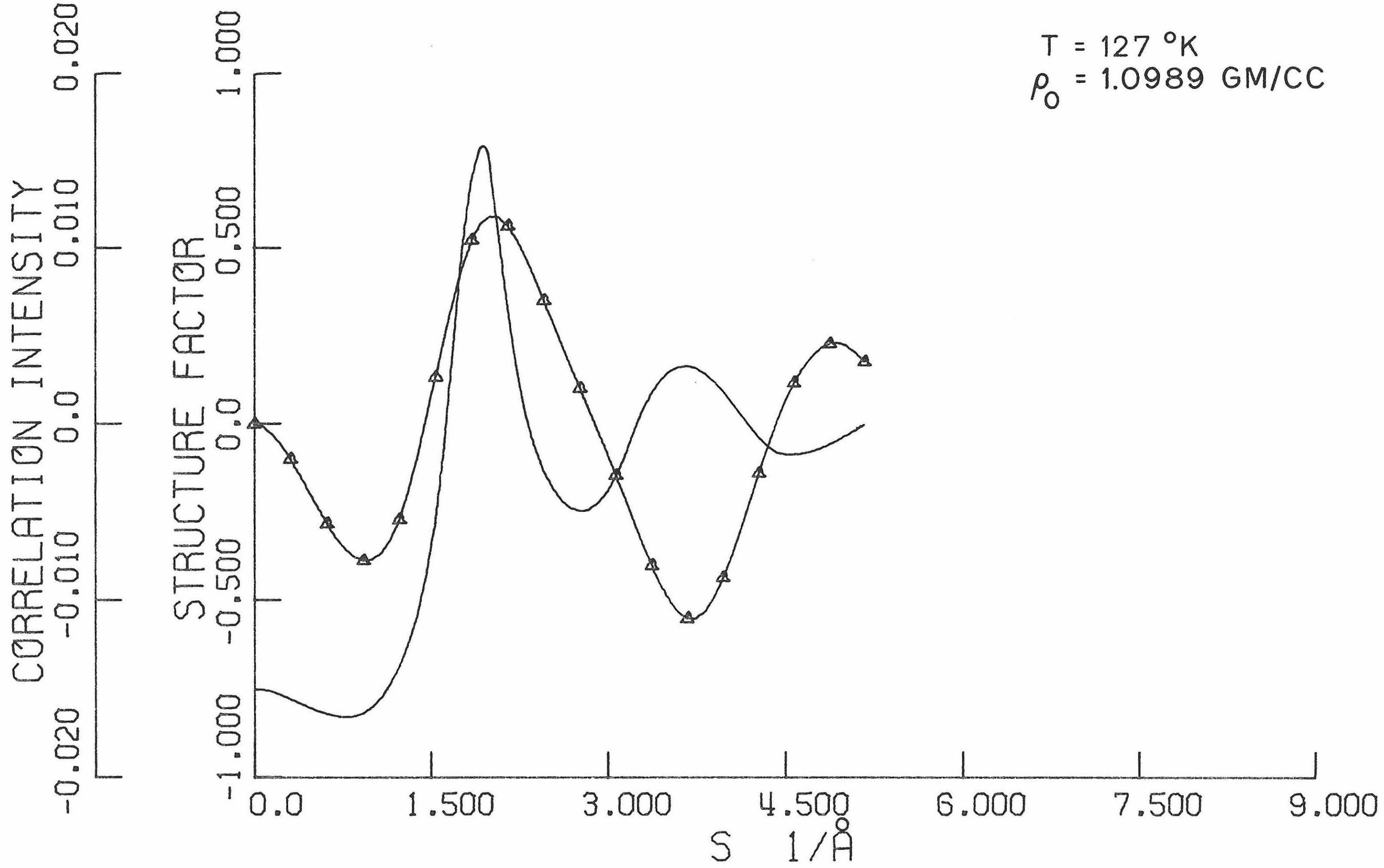

FIG. 23. —— STRUCTURE FACTOR FROM AR X-RAY DATA
-△△△- CORRECTION DUE TO CORRELATION

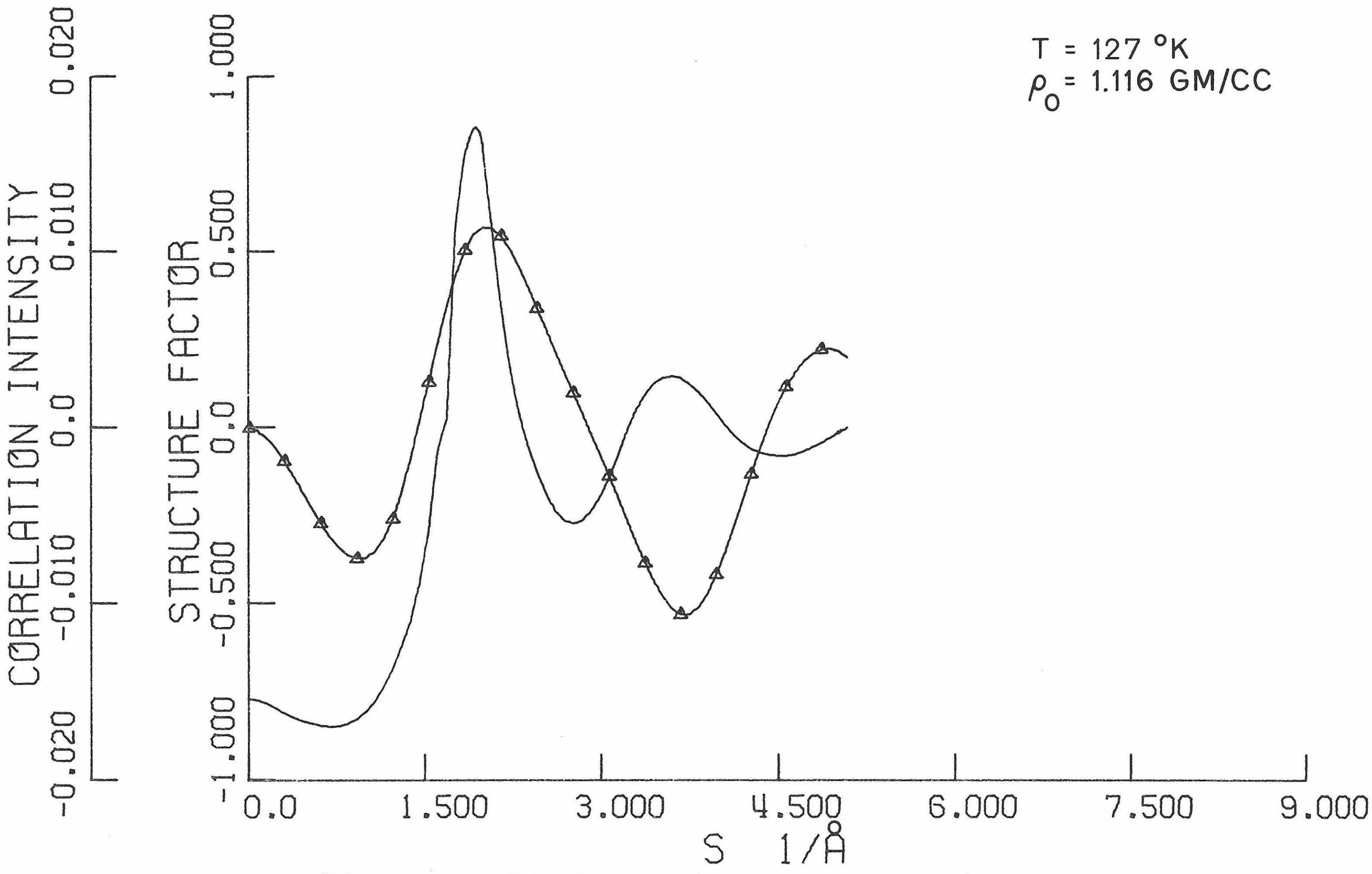

FIG. 24. —— STRUCTURE FACTOR FROM AR X-RAY DATA
-△-△-△- CORRECTION DUE TO CORRELATION

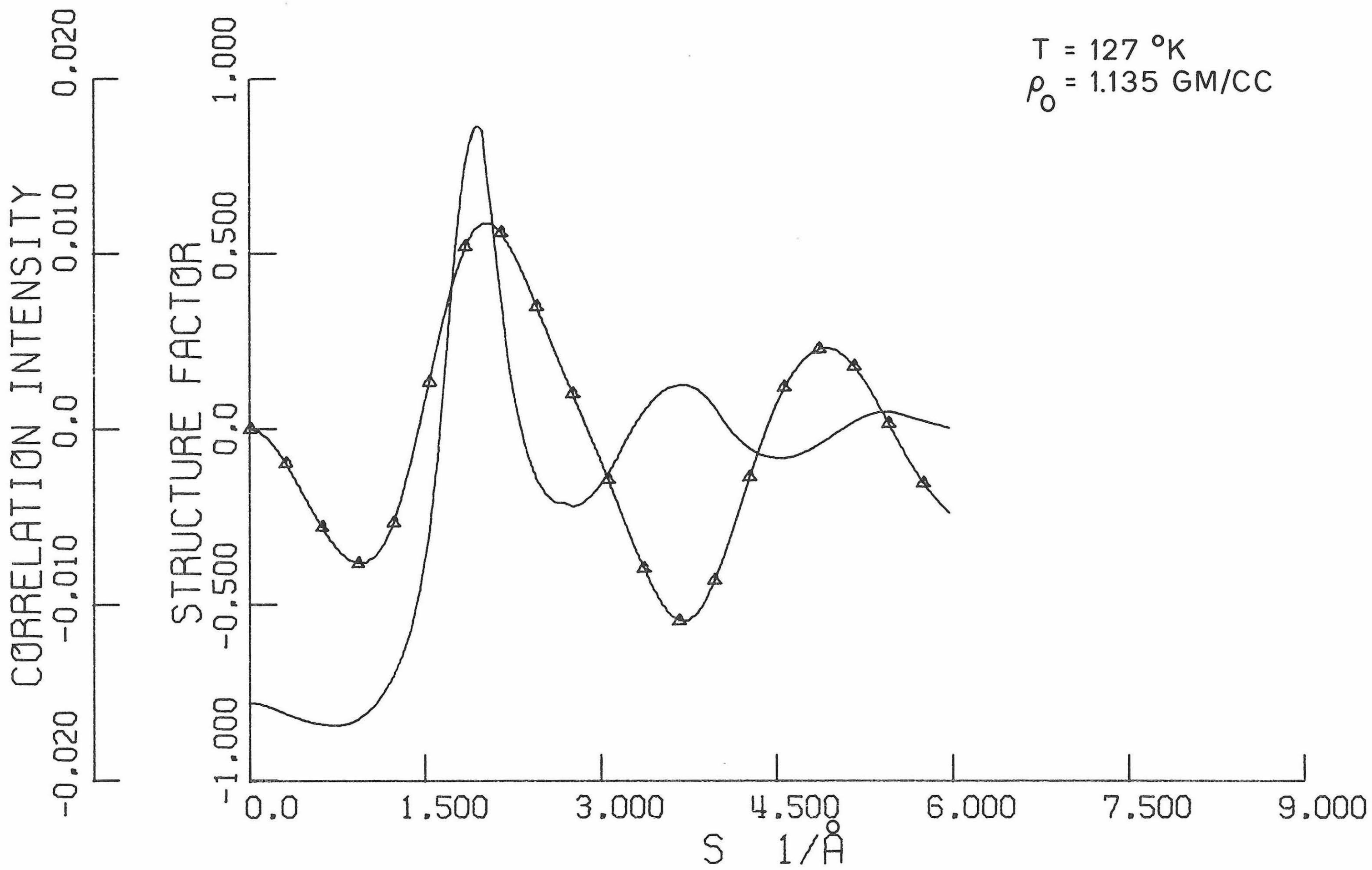

FIG. 25. —— STRUCTURE FACTOR FROM AR X-RAY DATA
△△△ CORRECTION DUE TO CORRELATION

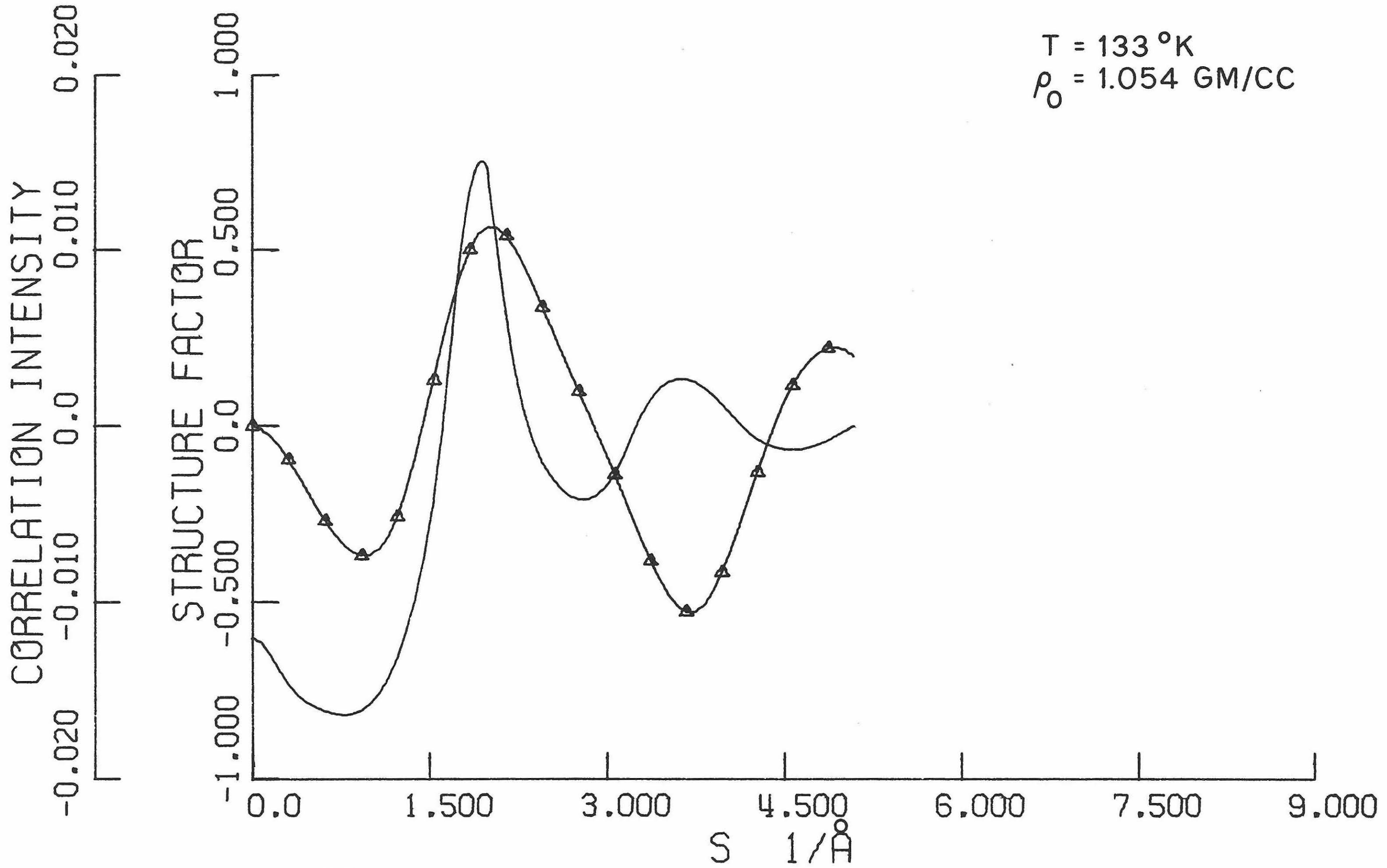

FIG. 26. ——— STRUCTURE FACTOR FROM AR X-RAY DATA
–△△△– CORRECTION DUE TO CORRELATION

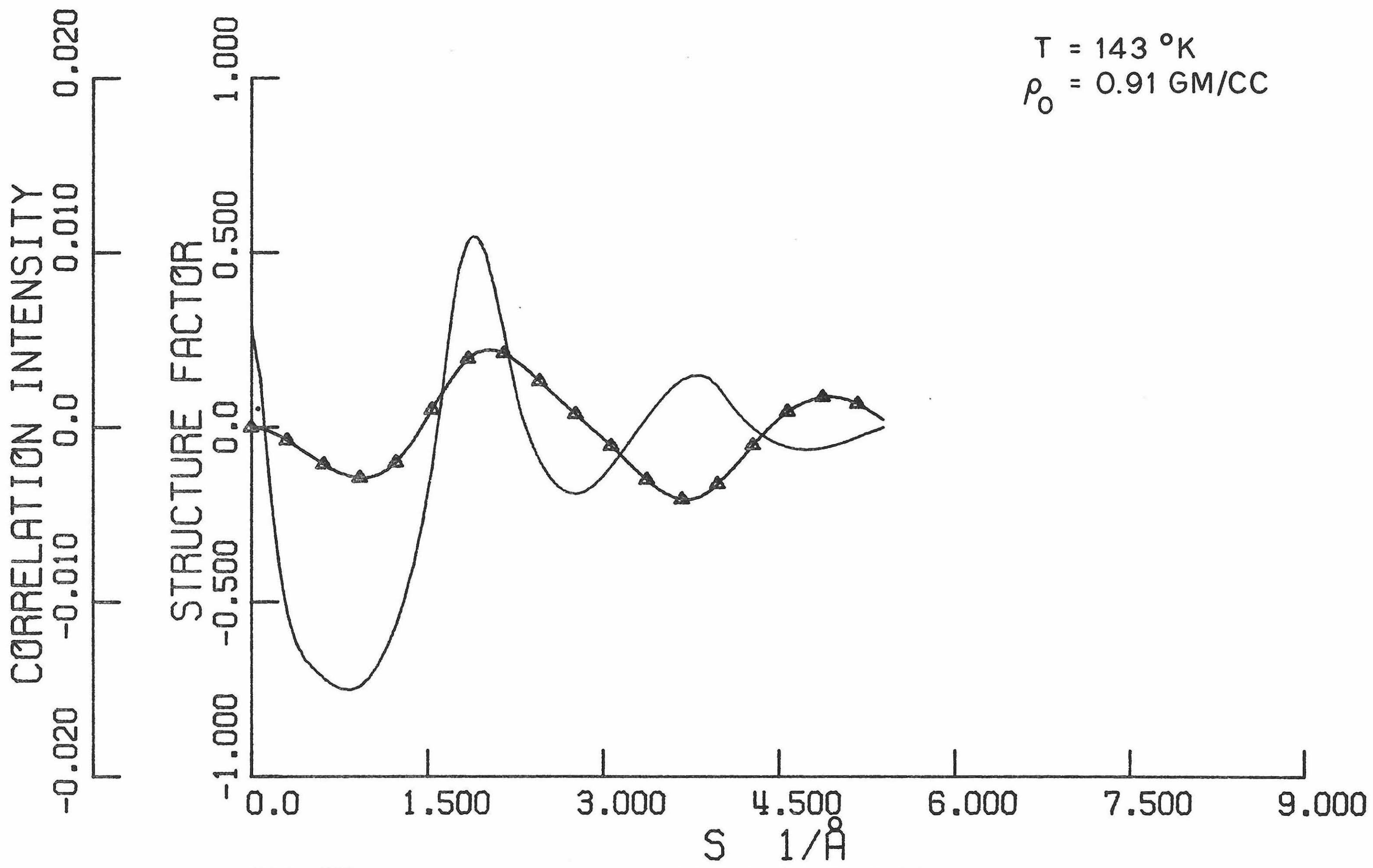

FIG. 27. —— STRUCTURE FACTOR FROM AR X-RAY DATA
△△△ CORRECTION DUE TO CORRELATION

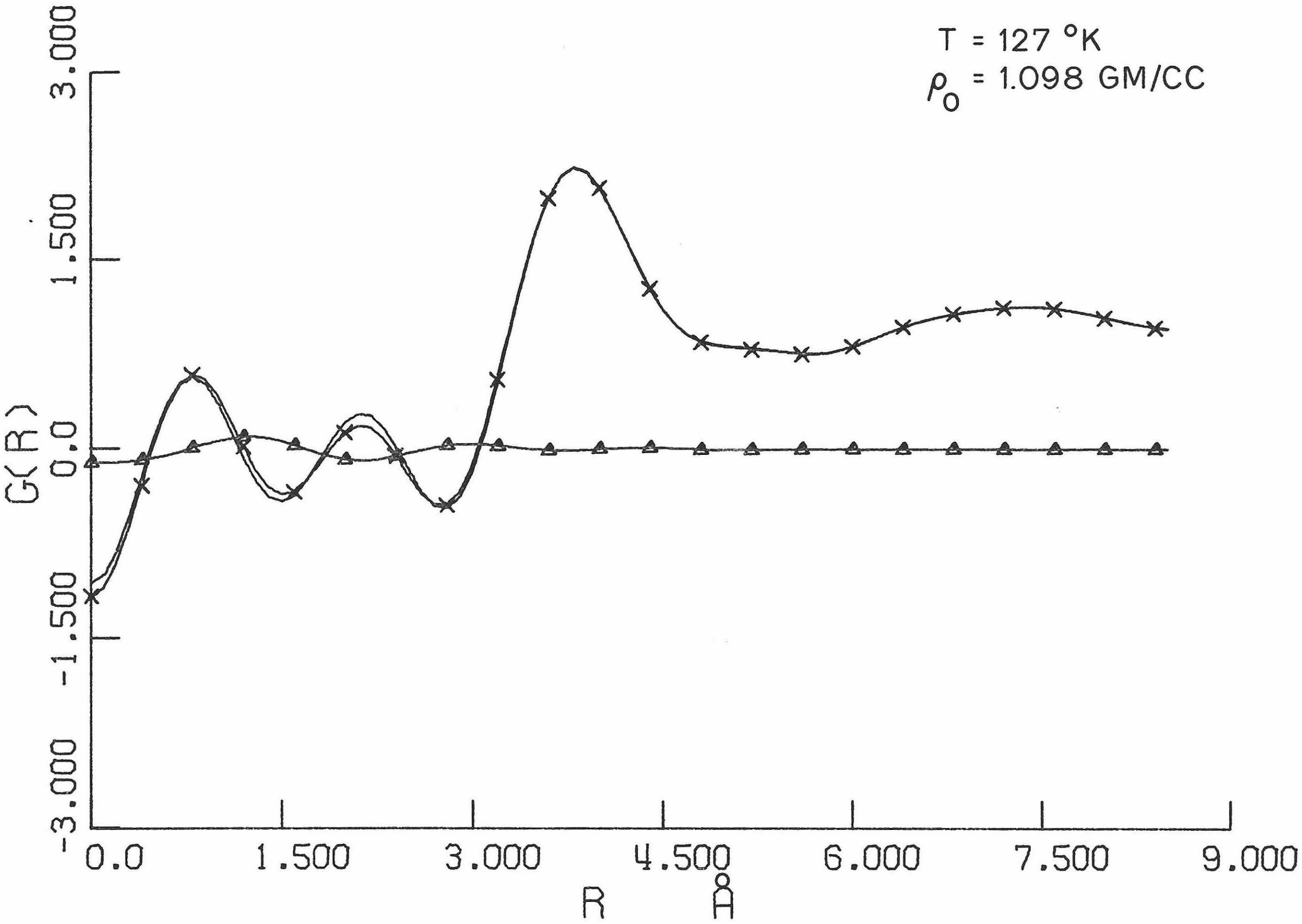

FIG. 28. RADIAL DISTRIBUTION FUNCTIONS FROM AR X-RAY DATA.
——— UNCORRELATED SCATTERING —×××— CORRELATED SCATTERING
—△△△— DEVIATION DUE TO CORRELATION

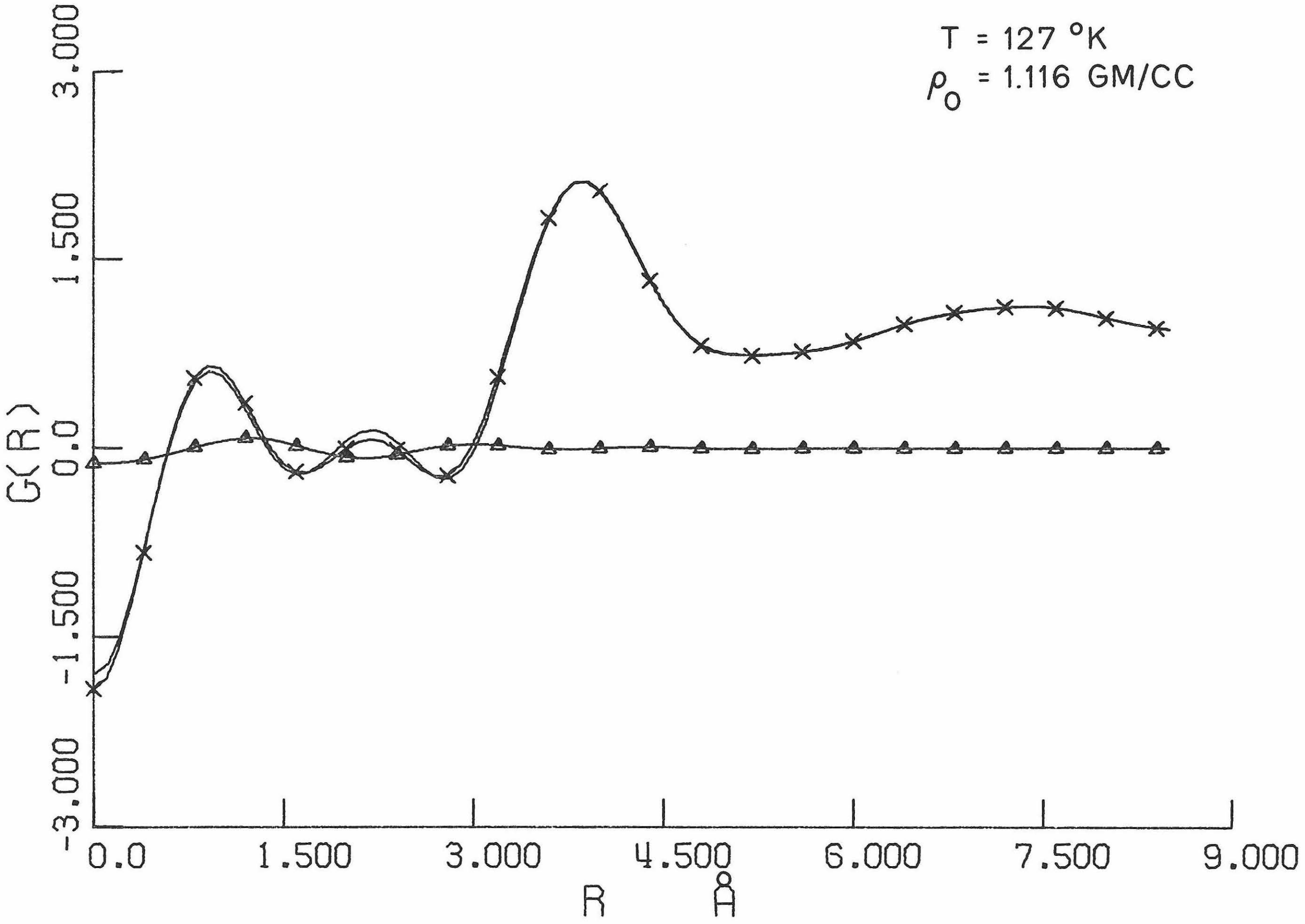

FIG. 29. RADIAL DISTRIBUTION FUNCTIONS FROM AR X-RAY DATA.
—— UNCORRELATED SCATTERING ✕✕✕ CORRELATED SCATTERING
△△△ DEVIATION DUE TO CORRELATION

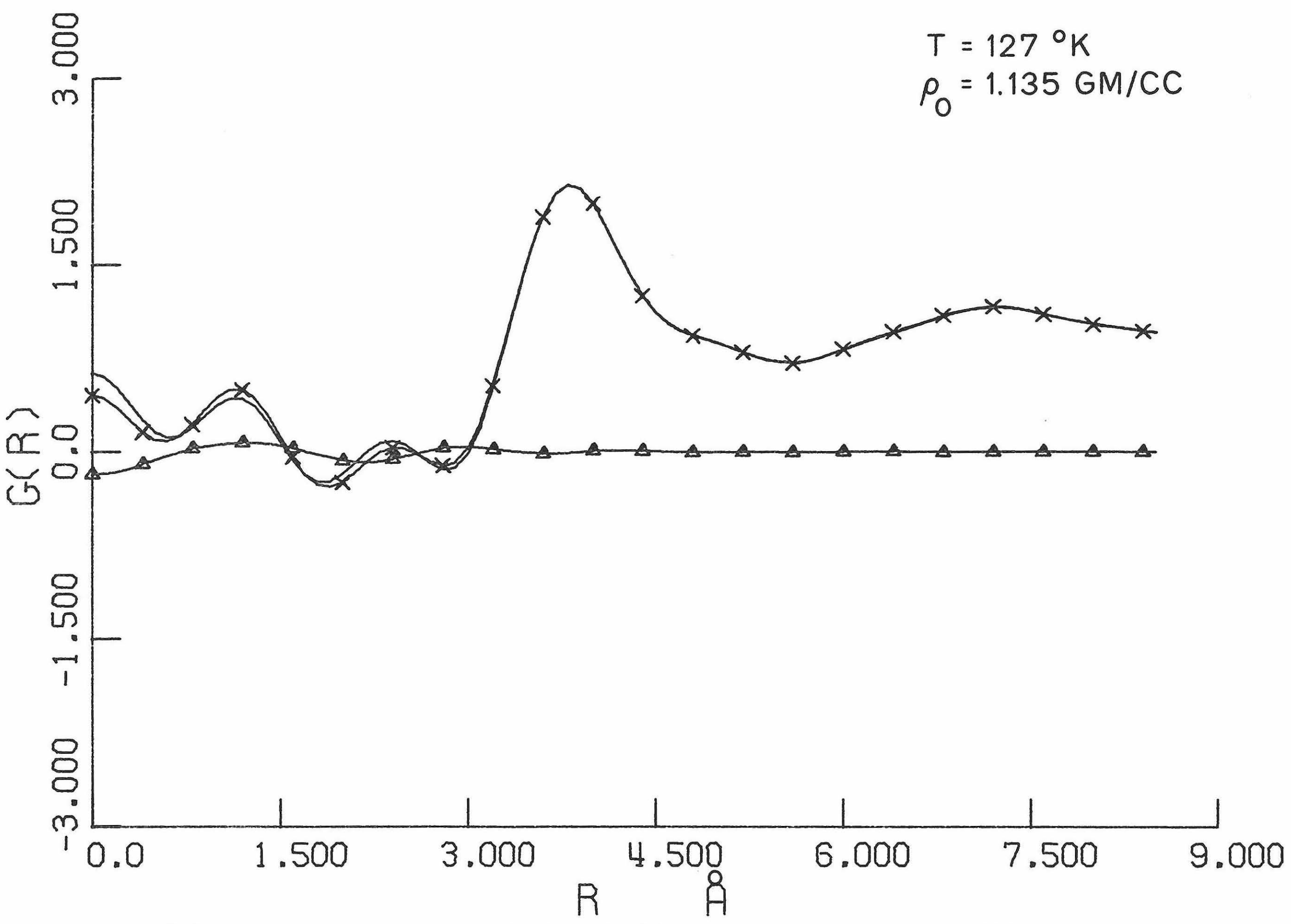

FIG. 30. RADIAL DISTRIBUTION FUNCTIONS FROM AR X-RAY DATA.

—— UNCORRELATED SCATTERING —×××— CORRELATED SCATTERING

—△△△— DEVIATION DUE TO CORRELATION

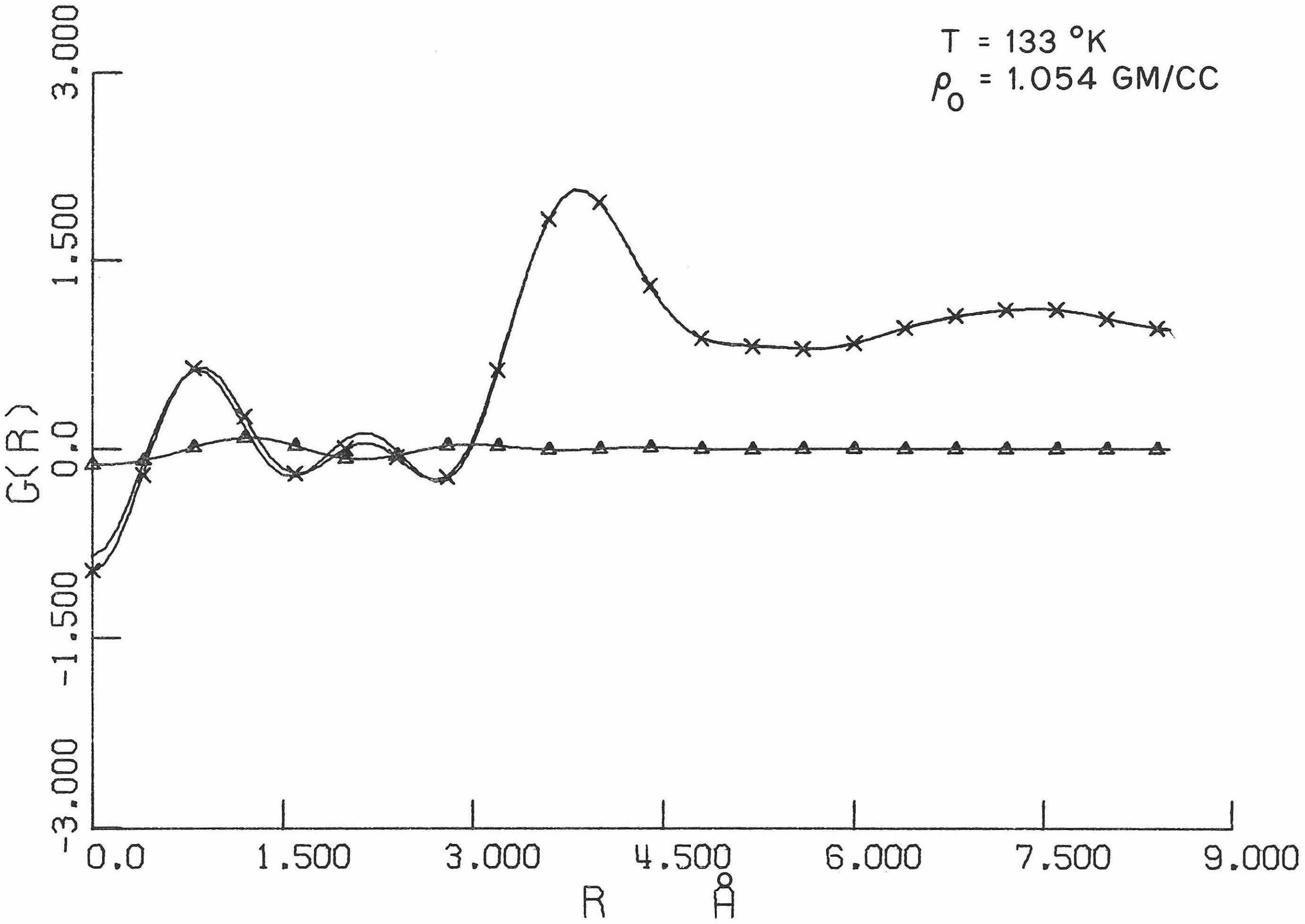

FIG. 31. RADIAL DISTRIBUTION FUNCTIONS FROM AR X-RAY DATA.
——— UNCORRELATED SCATTERING ✕✕✕ CORRELATED SCATTERING
△△△ DEVIATION DUE TO CORRELATION

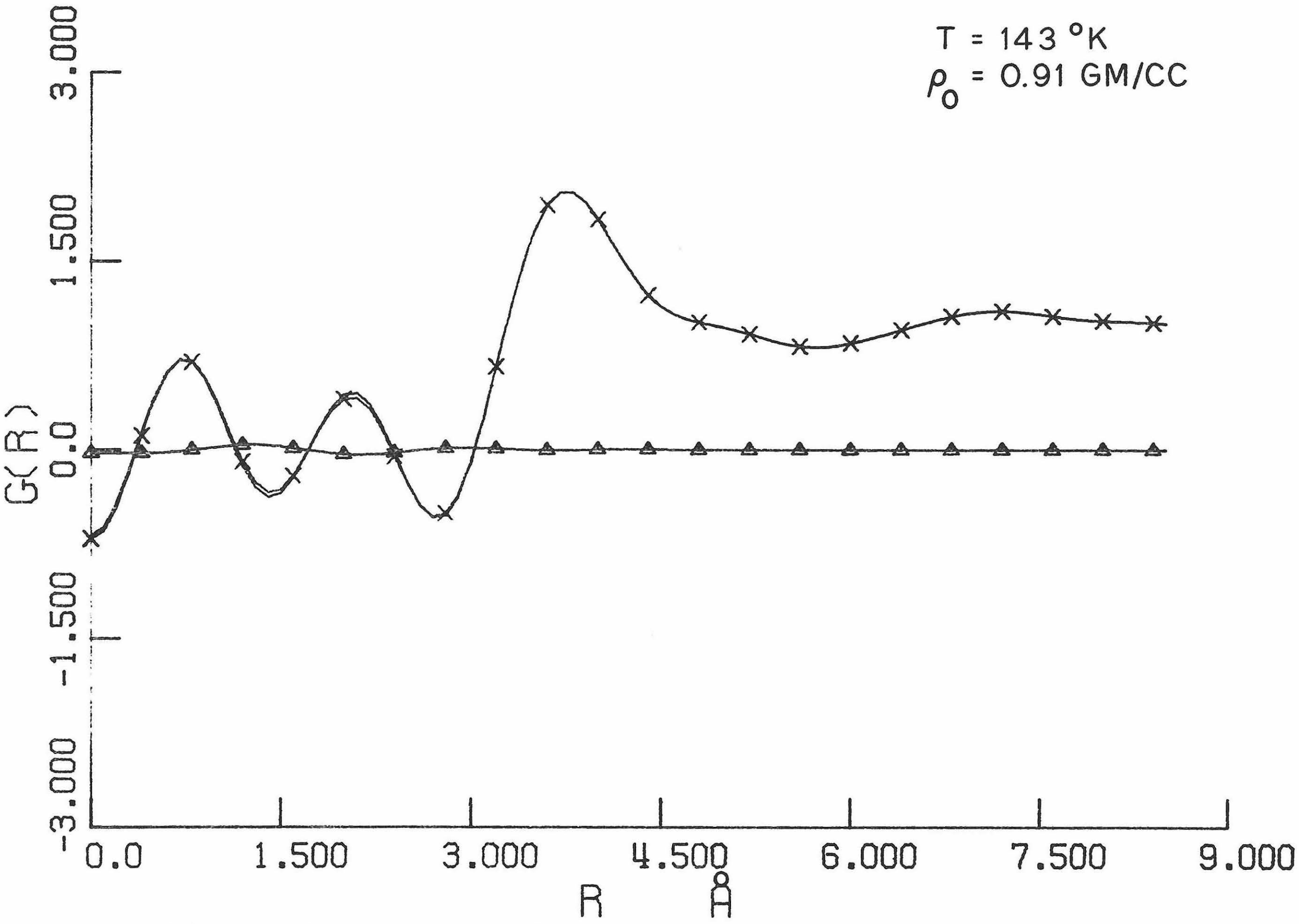

FIG. 32. RADIAL DISTRIBUTION FUNCTIONS FROM AR X-RAY DATA.

——— UNCORRELATED SCATTERING ✕✕✕ CORRELATED SCATTERING

△△△ DEVIATION DUE TO CORRELATION

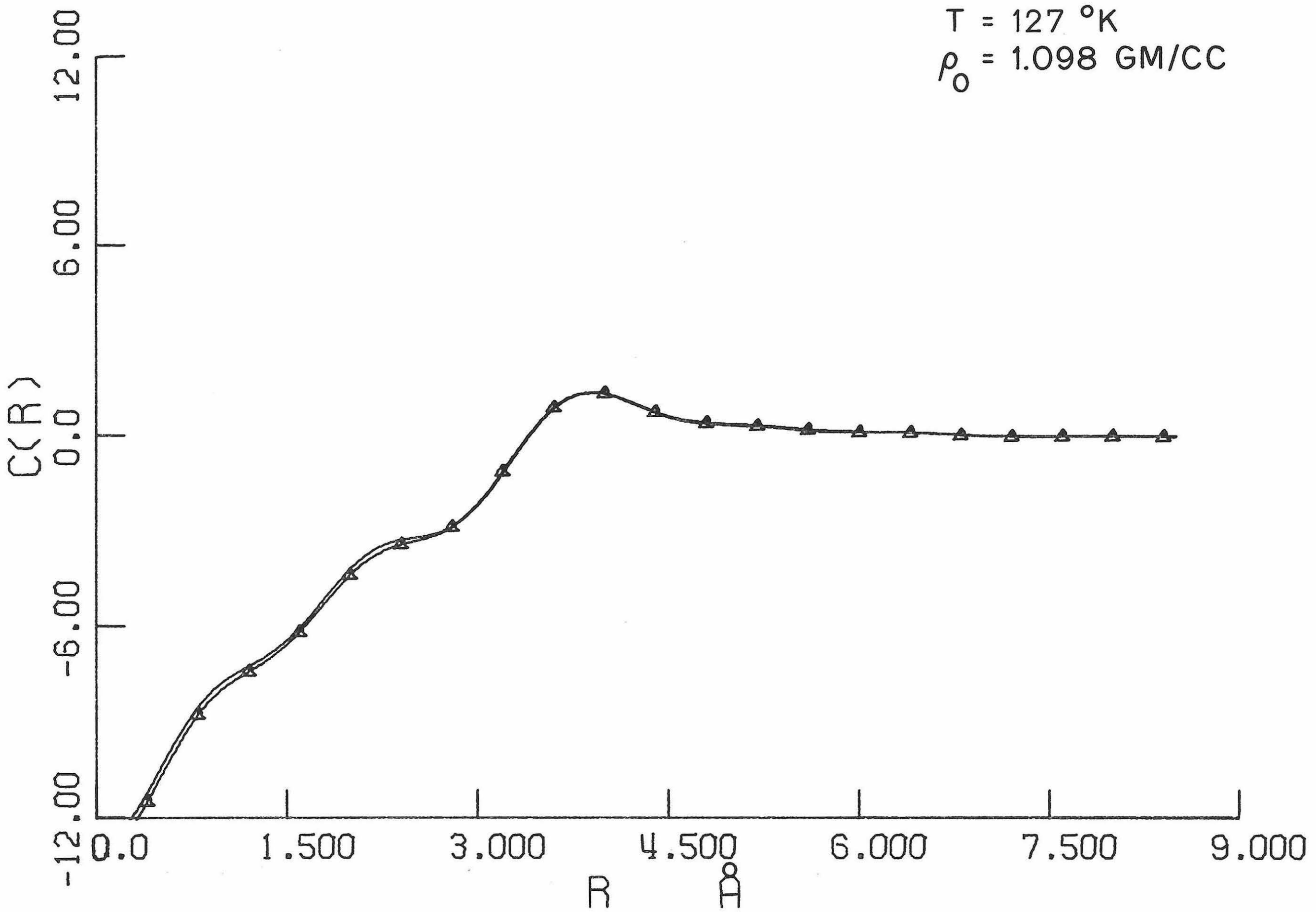

FIG. 33. DIRECT CORRELATION FUNCTIONS FROM AR X-RAY DATA.
——— UNCORRELATED SCATTERING -△△△- CORRELATED SCATTERING

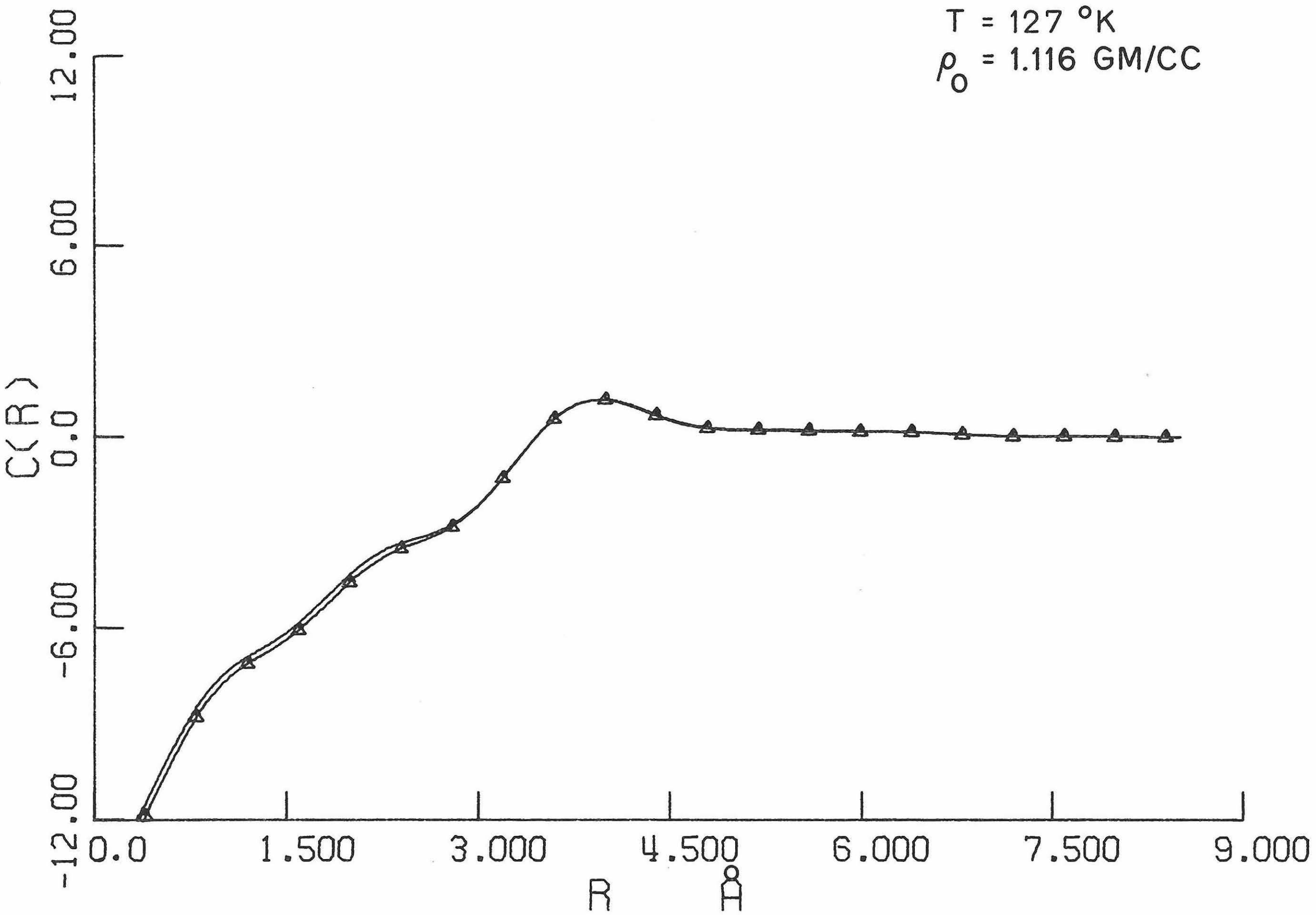

FIG. 34. DIRECT CORRELATION FUNCTIONS FROM AR X-RAY DATA.
——— UNCORRELATED SCATTERING —△△△— CORRELATED SCATTERING

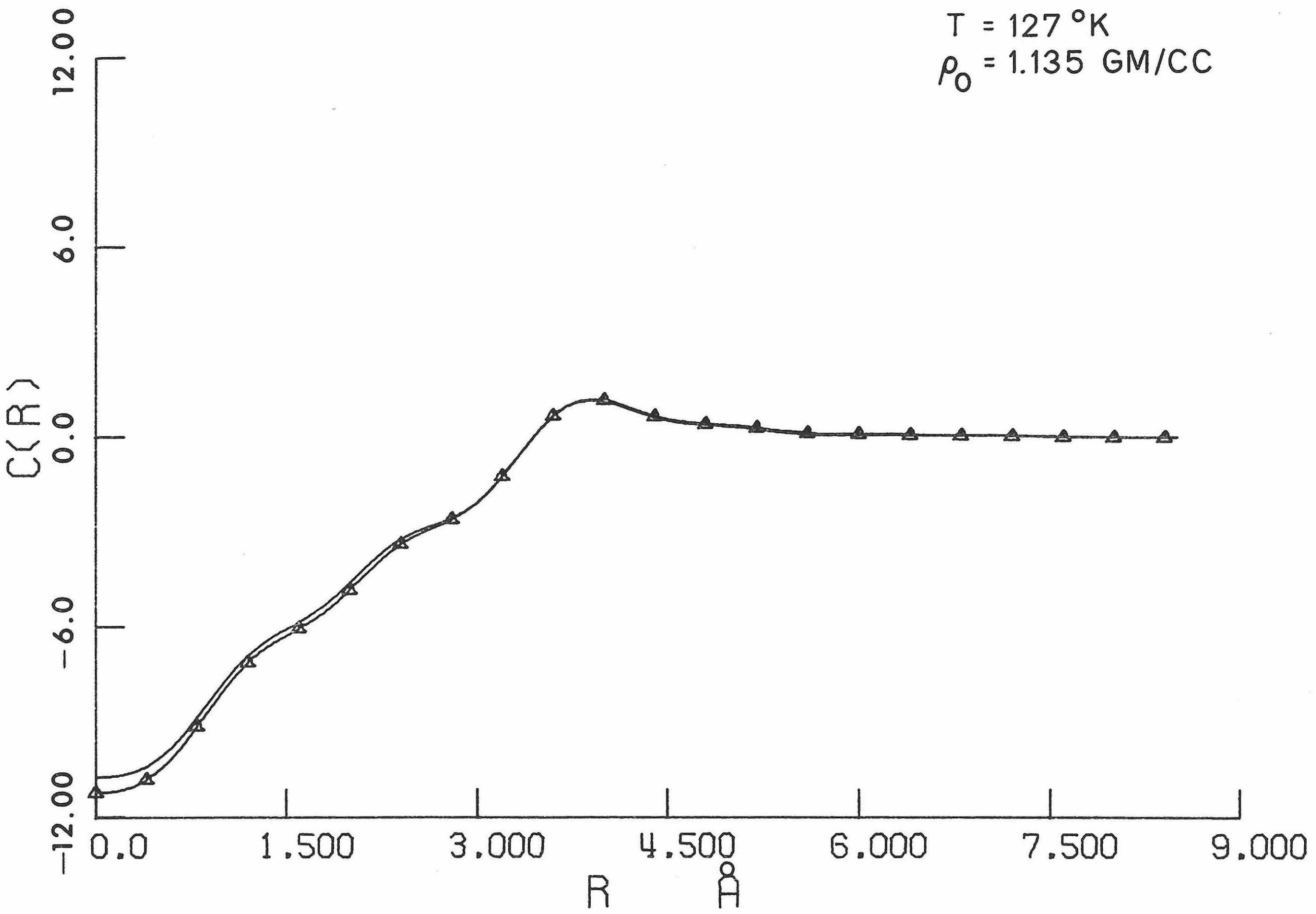

FIG. 35. DIRECT CORRELATION FUNCTIONS FROM AR X-RAY DATA.
—— UNCORRELATED SCATTERING -△-△-△- CORRELATED SCATTERING

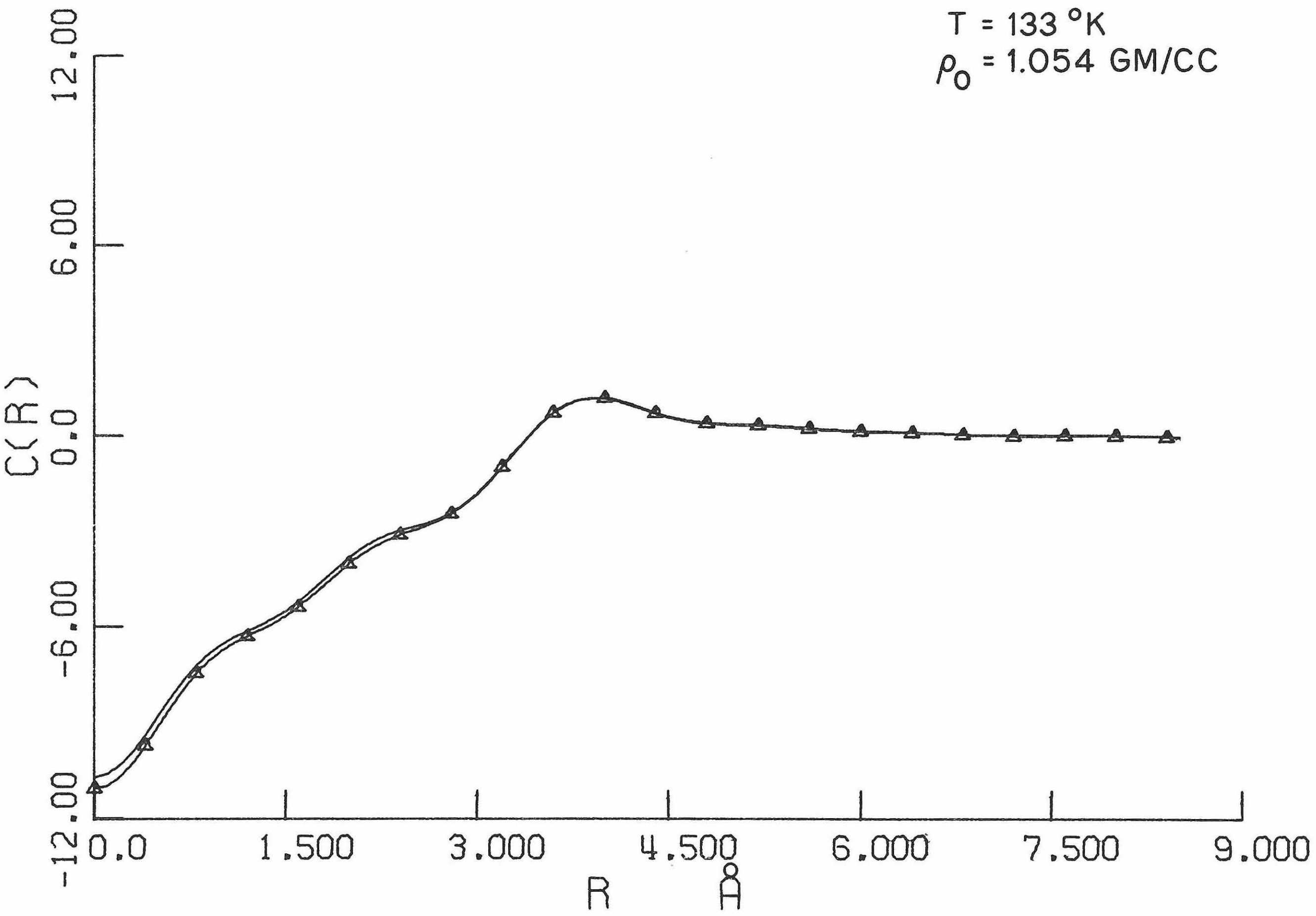

FIG. 36. DIRECT CORRELATION FUNCTIONS FROM AR X-RAY DATA.
—— UNCORRELATED SCATTERING -△△△- CORRELATED SCATTERING

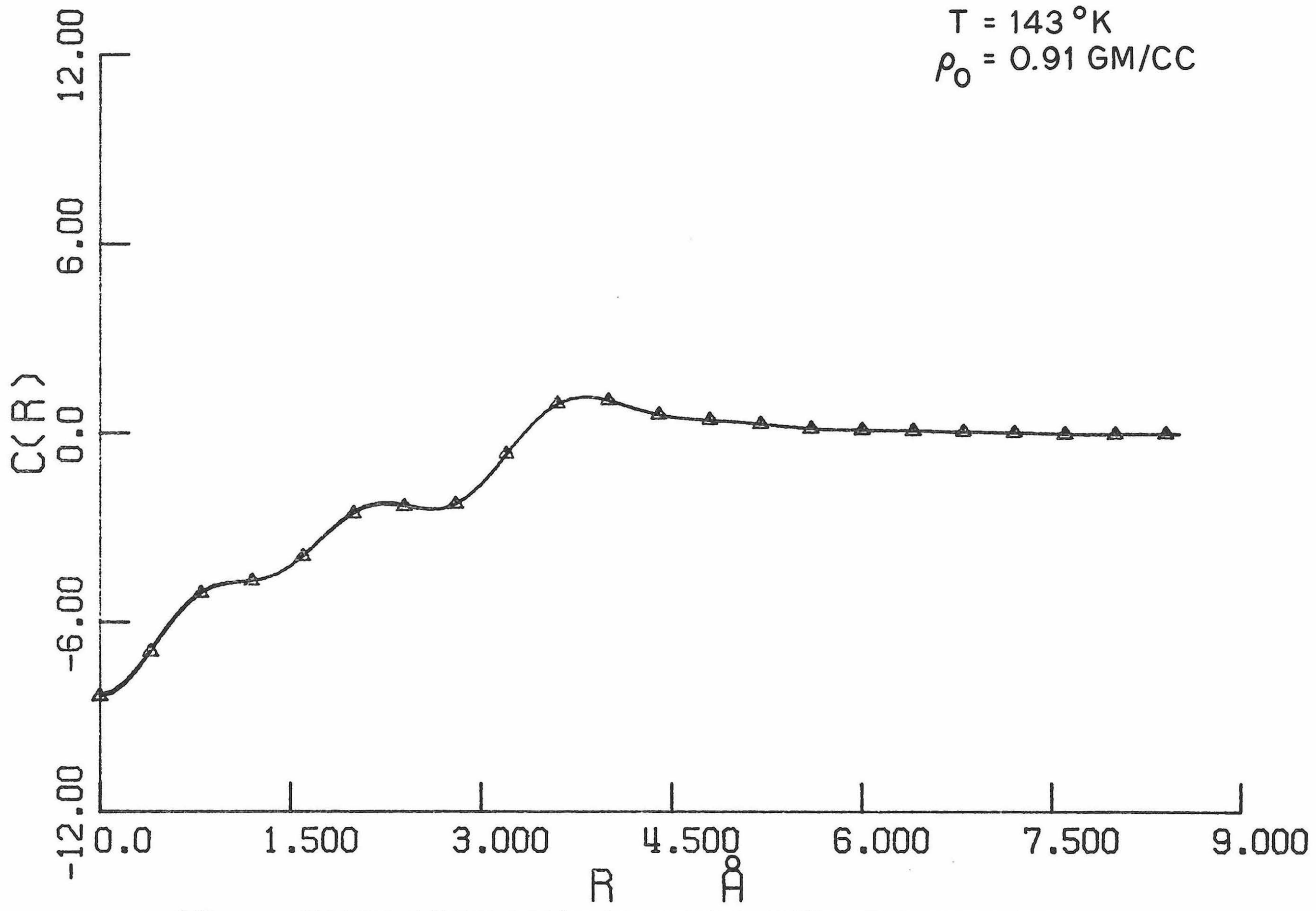

FIG. 37. DIRECT CORRELATION FUNCTIONS FROM AR X-RAY DATA.
—— UNCORRELATED SCATTERING —△—△—△— CORRELATED SCATTERING

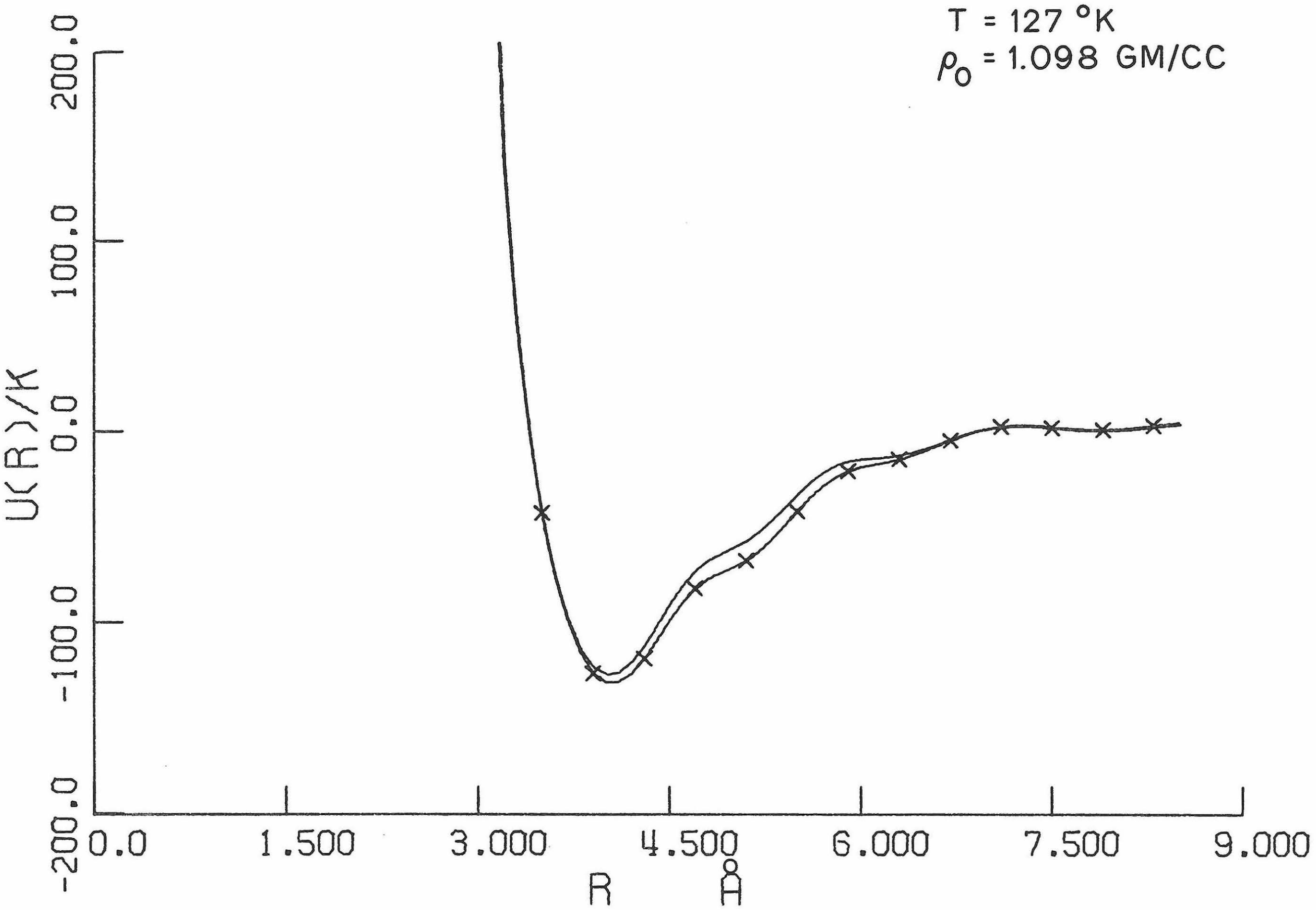

FIG. 38 INTERMOLECULAR ENERGY FOR ARGON FROM X-RAY DATA (PY THEORY).
——— UNCORRELATED SCATTERING ×××× CORRELATED SCATTERING

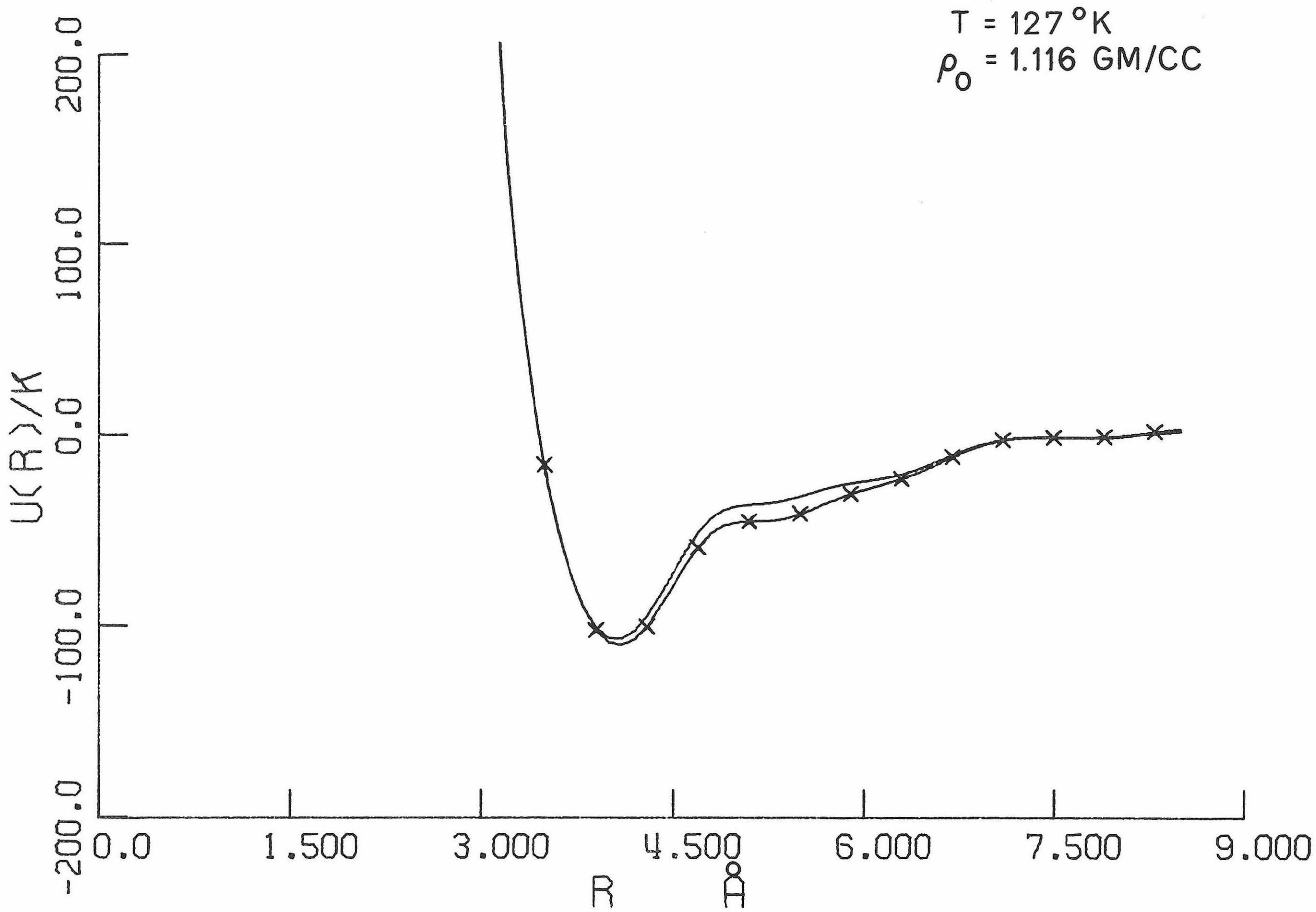

FIG. 39. INTERMOLECULAR ENERGY FOR ARGON FROM X-RAY DATA (PY THEORY).
——— UNCORRELATED SCATTERING —×—×—×— CORRELATED SCATTERING

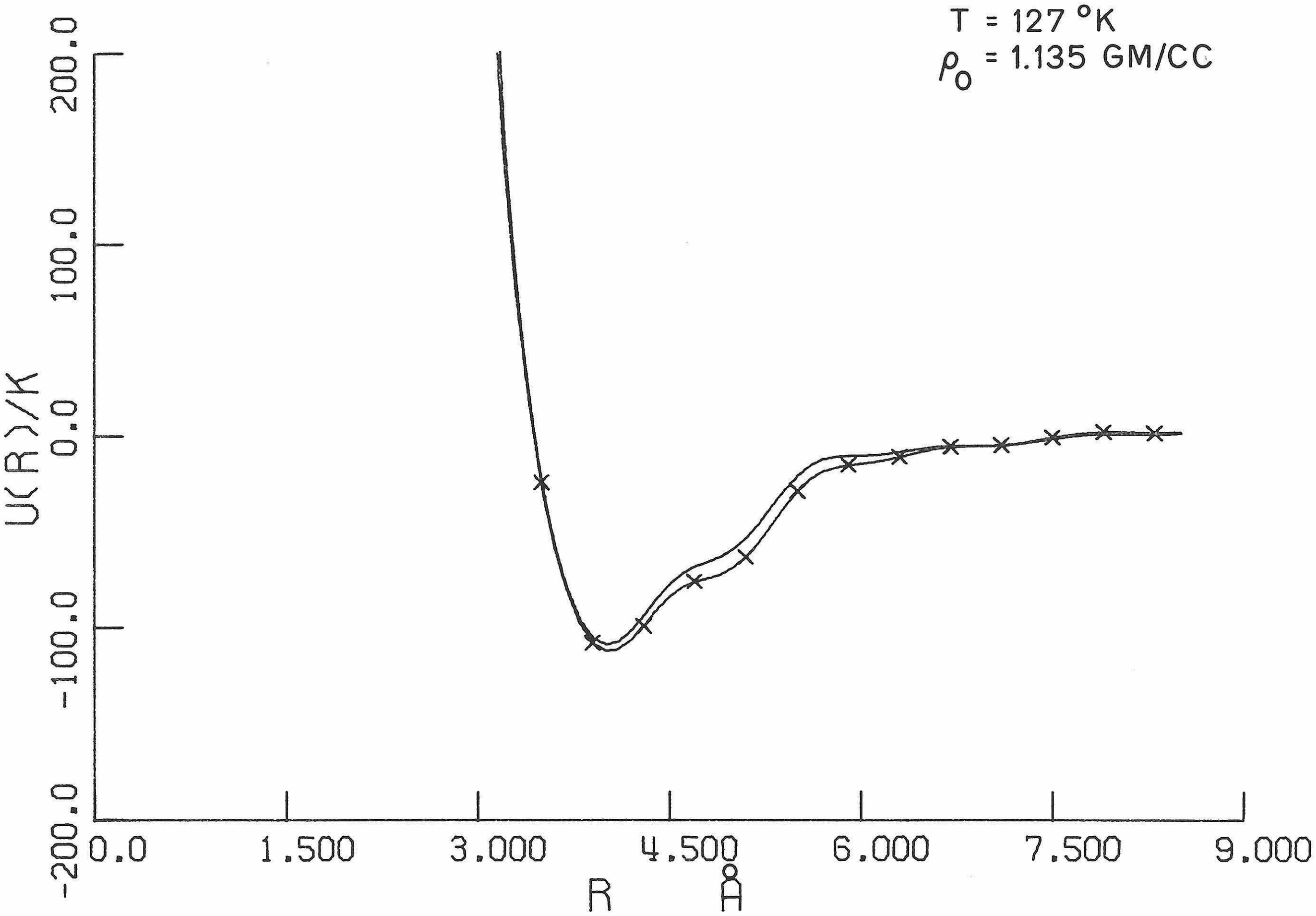

FIG. 40. INTERMOLECULAR ENERGY FOR ARGON FROM X-RAY DATA (PY THEORY).
—— UNCORRELATED SCATTERING ×××CORRELATED SCATTERING

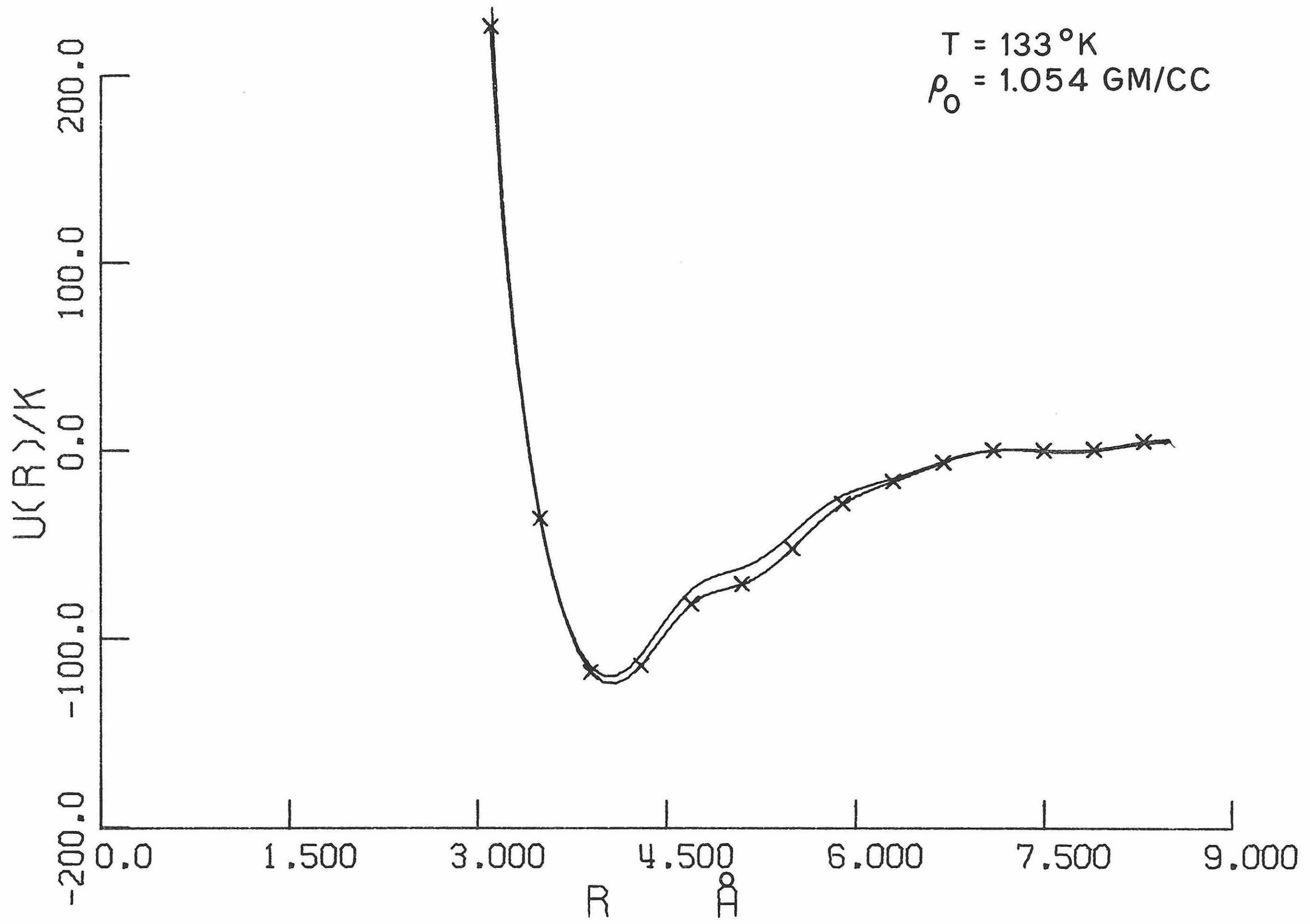

FIG. 41. INTERMOLECULAR ENERGY FOR ARGON FROM X-RAY DATA (PY THEORY).
—— UNCORRELATED SCATTERING -×-×-×- CORRELATED SCATTERING

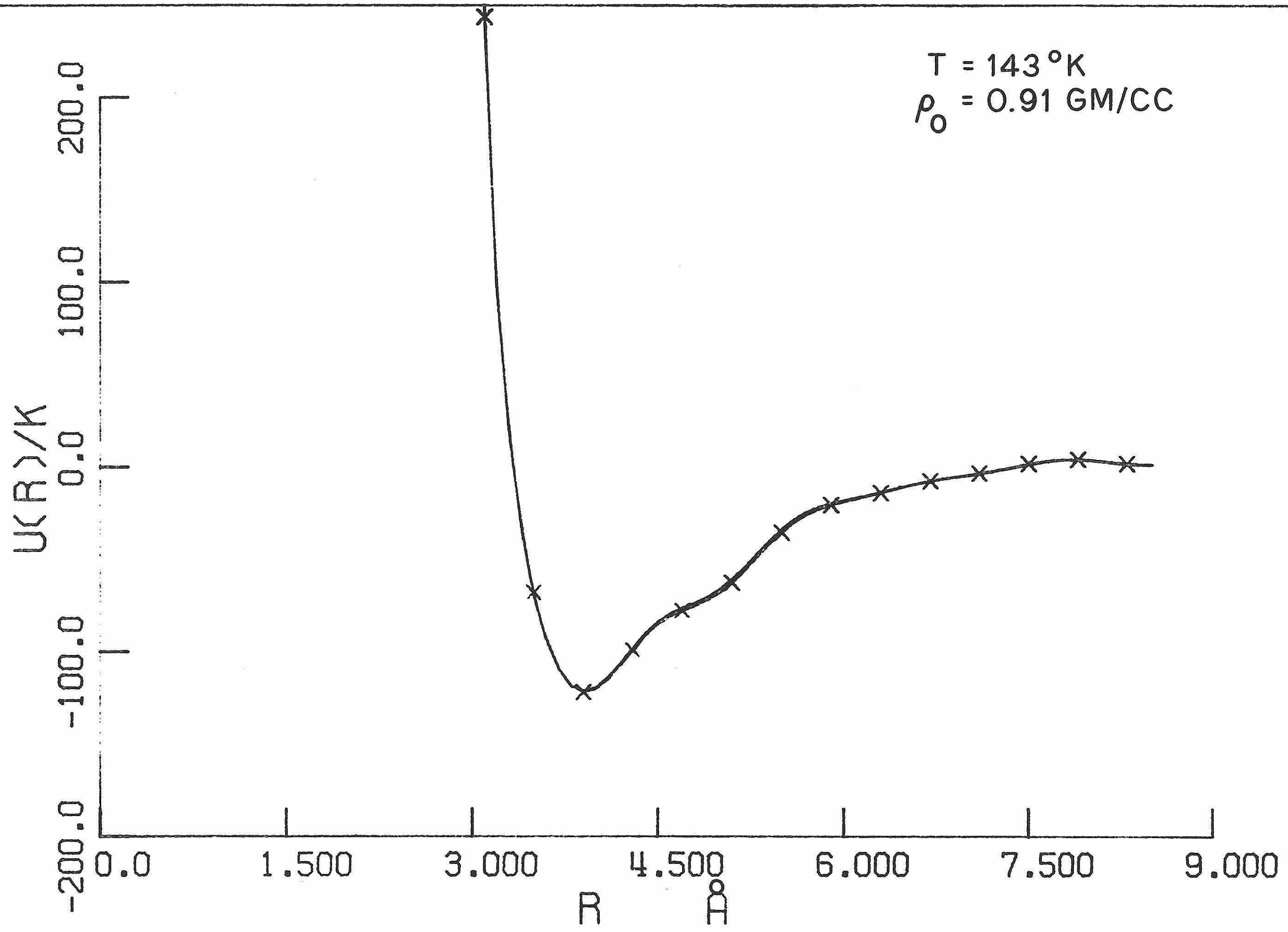

FIG. 42. INTERMOLECULAR ENERGY FOR ARGON FROM X-RAY DATA (PY THEORY).
—— UNCORRELATED SCATTERING ×××CORRELATED SCATTERING

Appendix D

<u>Tables 1 - 12</u>

TABLE 1

HELIUM CORRELATION AMPLITUDES
ORIENTATION ANGLE $(\bar{S}\cdot\bar{R}) = 0.0$

σ_g ORBITAL

R(au)	2.3622	3.7795	4.7244	5.1024	6.4252
SIN(θ)/λ $Å^{-1}$					
0.0	0.00000	0.00000	0.00000	0.00000	0.00000
0.1	0.02077	0.00469	0.00000	-0.00057	-0.00053
0.2	0.00000	-0.02389	-0.00944	-0.00517	-0.00014
0.3	-0.05848	-0.01208	0.00000	-0.00067	-0.00070
0.4	-0.05383	-0.00181	-0.00489	-0.00228	-0.00236
0.5	-0.01304	-0.00946	0.00000	-0.00077	-0.00004
0.6	-0.00000	-0.00047	-0.00239	-0.00078	-0.00028
0.7	-0.00824	-0.00301	0.00000	-0.00064	-0.00011
0.8	-0.00932	-0.00192	-0.00118	-0.00021	-0.00000
0.9	-0.00270	-0.00024	0.00000	-0.00045	-0.00009
1.0	0.00000	-0.00156	-0.00062	-0.00004	-0.00005
1.1	-0.00184	-0.00010	0.00000	-0.00029	0.00000
1.2	-0.00239	-0.00058	-0.00035	0.00000	-0.00004
1.3	-0.00079	-0.00042	0.00000	-0.00017	-0.00003
1.4	0.00000	-0.00005	-0.00022	0.00000	0.00000
1.5	-0.00058	-0.00040	0.00000	0.00000	0.00000

TABLE 2

HELIUM CORRELATION AMPLITUDE
ORIENTATION ANGLE $(\bar{S}\cdot\bar{R}) = 0.0$

σ_u ORBITAL

R(au)	2.3622	3.7798	4.7244	5.1024	6.4262
SIN(Θ)/λ $Å^{-1}$					
0.0	0.00000	0.00000	0.00000	0.00000	0.00000
0.1	-0.03007	-0.00493	0.00000	0.00057	0.00053
0.2	0.00000	0.02546	0.00938	0.00513	0.00014
0.3	0.09121	0.01315	0.00000	0.00067	0.00071
0.4	0.08880	0.00197	0.00479	0.00225	0.00024
0.5	0.02330	0.01057	0.00000	0.00076	0.00004
0.6	0.00000	0.00054	0.00231	0.00076	0.00028
0.7	0.01467	0.00343	0.00000	0.00063	0.00011
0.8	0.01763	0.00222	0.00114	0.00021	0.00001
0.9	0.00547	0.00027	0.00000	0.00044	0.00010
1.0	0.00000	0.00183	0.00060	0.00004	0.00006
1.1	0.00356	0.00011	0.00000	0.00028	0.00000
1.2	0.00484	0.00068	0.00034	0.00000	0.00004
1.3	0.00169	0.00049	0.00000	0.00017	0.00003
1.4	0.00000	0.00006	0.00019	0.00001	0.00000
1.5	0.00118	0.00047	0.00000	0.00009	0.00001

TABLE 3

HELIUM CORRELATION AMPLITUDES ORIENTATION ANGLE $(\bar{S}\cdot\bar{R}) = \pi/2$

σ_g ORBITAL

R(au) SIN(Θ)/λ $Å^{-1}$	2.3622	3.7795	4.7244	5.1024	6.4262
0.0	0.00000	0.00000	0.00000	0.00000	0.00000
0.1	-0.00366	-0.00242	-0.00108	-0.00073	-0.00016
0.2	-0.01101	-0.00683	-0.00299	-0.00199	-0.00044
0.3	-0.01613	-0.00915	-0.00389	-0.00256	-0.00054
0.4	-0.01701	-0.00880	-0.00364	-0.00237	-0.00047
0.5	-0.01503	-0.00717	-0.00292	-0.00189	-0.00038
0.6	-0.01204	-0.00538	-0.00217	-0.00140	-0.00029
0.7	-0.00916	-0.00391	-0.00157	-0.00101	-0.00021
0.8	-0.00680	-0.00281	-0.00113	-0.00073	-0.00015
0.9	-0.00502	-0.00204	-0.00082	-0.00053	-0.00011
1.0	-0.00371	-0.00149	-0.00061	-0.00039	-0.00008
1.1	-0.00277	-0.00111	-0.00045	-0.00029	-0.00006
1.2	-0.00210	-0.00084	-0.00034	-0.00022	-0.00005
1.3	-0.00161	-0.00064	-0.00026	-0.00017	-0.00004
1.4	-0.00125	-0.00050	-0.00021	-0.00014	-0.00003
1.5	-0.00098	-0.00039	-0.00016	-0.00010	-0.00002

TABLE 4

HELIUM CORRELATION AMPLITUDE
ORIENTATION ANGLE $(\bar{S}\cdot\bar{R}) = \pi/2$

σ_u ORBITAL

R(au) SIN(Θ)/λ $Å^{-1}$	2.3622	3.7798	4.7244	5.1024	6.4262
0.0	0.00000	0.00000	0.00000	0.00000	0.00000
0.1	0.00826	0.00273	0.00107	0.00073	0.00017
0.2	0.02439	0.00769	0.00292	0.00196	0.00044
0.3	0.03503	0.01036	0.00379	0.00253	0.00055
0.4	0.03632	0.01003	0.00355	0.00234	0.00050
0.5	0.03169	0.00821	0.00283	0.00186	0.00039
0.6	0.02522	0.00620	0.00210	0.00138	0.00029
0.7	0.01915	0.00453	0.00152	0.00100	0.00021
0.8	0.01425	0.00328	0.00110	0.00072	0.00015
0.9	0.01056	0.00239	0.00080	0.00053	0.00011
1.0	0.00786	0.00176	0.00059	0.00039	0.00008
1.1	0.00590	0.00131	0.00044	0.00029	0.00006
1.2	0.00448	0.00099	0.00033	0.00022	0.00005
1.3	0.00344	0.00076	0.00025	0.00017	0.00004
1.4	0.00267	0.00058	0.00019	0.00012	0.00002
1.5	0.00211	0.00046	0.00015	0.00010	0.00002

TABLE 5

ORIENTATIONAL AVERAGE OF HELIUM CORRELATION AMPLITUDES

σ_g ORBITAL

R(au) $\mathrm{SIN}(\Theta)/\lambda$ $\mathrm{\AA}^{-1}$	2.3622	3.7798	4.7244	5.1024	6.4262
0.0	0.00000	0.00000	0.00000	0.00000	0.00000
0.2	-0.00734	-0.01252	-0.00514	-0.00305	-0.00034
0.4	-0.02929	-0.00647	-0.00406	-0.00234	-0.00040
0.6	-0.00803	-0.00374	-0.00224	-.000120	-0.00028
1.0	-0.00247	-0.00152	-0.00061	-0.00027	-0.00007
1.4	-0.00084	-0.00035	-0.00021	-0.00009	-0.00002

TABLE 6

ORIENTATIONAL AVERAGE OF HELIUM CORRELATION AMPLITUDES

σ_u ORBITAL

R(au)	2.3622	3.7798	4.7244	5.1024	6.4262
SIN(Θ)/λ Å^{-1}					
0.0	0.00000	0.00000	0.00000	0.00000	0.00000
0.2	0.01626	0.01362	0.00507	0.00302	0.00034
0.4	0.05381	0.00734	0.00396	0.00231	0.00041
0.6	0.01681	0.00431	0.00217	0.00117	0.00028
1.0	0.00524	0.00178	0.00059	0.00027	0.00007
1.4	0.00178	0.00041	0.00019	0.00008	0.00002

TABLE 7

ORIENTATIONALLY AVERAGED NET ORBITAL CORRELATION AMPLITUDES FOR HELIUM

R(au)	2.3622	3.7798	4.7244	5.1024	6.4262
SIN(Θ)/λ Å^{-1}					
0.0	0.00000	0.00000	0.00000	0.00000	0.00000
0.2	0.00892	0.00110	-0.00007	-0.00003	0.00000
0.4	0.02453	0.00087	-0.00010	-0.00003	0.00001
0.6	0.00878	0.00057	-0.00007	-0.00002	0.00000
0.8	0.00774	0.00041	-0.00004	-0.00001	0.00000
1.0	0.00276	0.00026	-0.00002	0.00000	0.00000
1.2	0.00241	0.00014	-0.00001	0.00000	0.00000
1.4	0.00094	0.00006	-0.00002	-0.00001	-0.00001

TABLE 8

RATIO OF NET ORBITAL CORRELATION AMPLITUDE TO ISOLATED HELIUM ATOM AMPLITUDE

R(au) $\mathrm{SIN}(\Theta)/\lambda$ $\mathrm{\AA}^{-1}$	2.3622	3.7798	4.7244	5.1024	6.4262
0.0	0.00000	0.00000	0.00000	0.00000	0.00000
0.2	0.01191	0.00146	-0.00009	-0.00004	0.00000
0.4	0.06446	0.000230	-0.00025	-0.00008	0.00002
0.6	0.05050	0.00329	-0.00043	-0.00014	0.00000
0.8	0.09395	0.00501	-0.00048	-0.00012	0.00001
1.0	0.06585	0.00629	-0.00050	-0.00011	0.00003
1.2	0.10455	0.00590	-0.00053	-0.00010	0.00003
1.4	0.06998	0.00417	-0.00143	-0.00070	-0.00056

TABLE 9

STRUCTURE FACTORS AND CORRELATION INTENSITIES FOR HELIUM

S ($Å^{-1}$)	T = 1.4 °K		T = 4.2 °K	
	STRUCTURE FACTOR	CORRELATION INTENSITY $\times 10^{-3}$	STRUCTURE FACTOR	CORRELATION INTENSITY $\times 10^{-3}$
0.000	-0.948	0.00	-0.525	0.00
0.100	-0.942	0.00	-0.580	0.00
0.200	-0.930	-0.02	-0.655	-0.02
0.300	-0.913	-0.05	-0.723	-0.04
0.400	-0.896	-0.08	-0.750	-0.07
0.500	-0.875	-0.11	-0.761	-0.09
0.750	-0.820	-0.16	-0.749	-0.14
1.000	-0.742	-0.13	-0.675	-0.11
1.250	-0.624	0.46	-0.554	0.05
1.500	-0.427	0.38	-0.346	0.35
1.700	-0.140	0.71	-0.071	0.63
1.800	0.070	0.86	0.094	0.77
1.900	0.255	0.99	0.247	0.88
2.000	0.417	1.10	0.349	0.98
2.100	0.374	1.17	0.330	1.04
2.200	0.268	1.20	0.224	1.07
2.300	0.190	1.17	0.143	1.04
2.500	0.072	0.92	0.044	0.82
2.750	-0.010	0.10	-0.014	0.16
3.000	-0.048	-0.93	-0.038	-0.84
3.250	-0.052	-2.27	-0.045	-2.04
3.500	-0.055	-3.71	-0.043	-3.32
3.750	-0.040	-5.09	-0.036	-4.56
4.000	-0.025	-6.29	-0.025	-5.63

TABLE 9 (continued)

STRUCTURE FACTORS AND CORRELATION INTENSITIES FOR HELIUM

S $\mathring{A}^{-1}$	T = 1.4 °K		T = 4.2 °K	
	STRUCTURE FACTOR	CORRELATION INTENSITY $\times 10^{-3}$	STRUCTURE FACTOR	CORRELATION INTENSITY $\times 10^{-3}$
4.250	-0.012	-7.25	-0.012	-6.49
4.500	-0.003	-7.93	-0.003	-7.10
4.750	0.000	-8.30	0.000	-7.43
5.000	0.000	-8.32	0.000	-7.45
5.250	0.000	-7.97	0.000	-7.13
5.650	0.000	-6.70	0.000	-6.00
6.000	0.000	-5.04	0.000	-4.51
6.450	0.000	-2.35	0.000	-2.12
6.600	0.000	-1.25	0.000	-1.20
6.900	0.000	-0.63	0.000	-0.62
7.350	0.000	-0.25	0.000	-0.26
7.800	0.000	-0.01	0.000	-0.01
8.200	0.000	0.00	0.000	0.00
8.600	0.000	0.00	0.000	0.00
9.000	0.000	0.00	0.000	0.00

TABLE 10

COMPARISON OF HELIUM PROPERTIES

T= 1.40 ^{0}K RHO=0.0218 ATOMS/Å^{3}

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K DIFFERENCE
0.0	-0.93398	-2.13236	-7.51822	-8.74381	
0.10000	-0.90697	-2.04992	-7.47914	-8.64862	
0.20000	-0.82850	-1.81524	-7.36463	-8.37591	
0.30000	-0.70596	-1.46353	-7.18288	-7.96195	
0.40000	-0.55077	-1.04540	-6.94647	-7.45888	
0.50000	-0.37714	-0.61688	-6.67121	-6.92470	
0.60000	-0.20061	-0.22908	-6.37452	-6.41282	
0.70000	-0.03636	0.08005	-6.07369	-5.96365	
0.80000	0.10230	0.29032	-5.78427	-5.59984	
0.90000	0.20528	0.39963	-5.51864	-5.32590	
1.00000	0.26659	0.42067	-5.28501	-5.13134	
1.10000	0.28484	0.37536	-5.08689	-4.99628	
1.20000	0.26318	0.28872	-4.92310	-4.89751	
1.30000	0.20877	0.18383	-4.78826	-4.81355	
1.40000	0.13186	0.07872	-4.67369	-4.72776	
1.50000	0.04458	-0.01452	-4.56863	-4.62928	
1.60000	-0.04039	-0.08889	-4.46162	-4.51224	
1.70000	-0.11111	-0.14074	-4.34175	-4.37395	
1.80000	-0.15758	-0.16795	-4.19994	-4.21318	
1.90000	-0.17253	-0.16873	-4.02972	-4.02896	
2.00000	-0.15196	-0.14134	-3.82786	-3.82031	
2.10000	-0.09532	-0.08457	-3.59446	-3.58669	

TABLE 10 (CONTINUED)

COMPARISON OF HELIUM PROPERTIES

T= 1.40 °K RHO=0.0218 ATOMS/Å^3

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K DIFFERENCE
2.20000	-0.00519	0.00148	-3.33275	-3.32888	
2.30000	0.11314	0.11452	-3.04859	-3.04975	
2.40000	0.25249	0.24979	-2.74970	-2.75463	
2.50000	0.40457	0.40025	-2.44478	-2.45101	
2.60000	0.56091	0.55741	-2.14271	-2.14782	
2.70000	0.71355	0.71242	-1.85170	-1.85419	
2.80000	0.85569	0.85724	-1.57874	-1.57838	
2.90000	0.98207	0.98554	-1.32913	-1.32678	
3.00000	1.08919	1.09322	-1.10635	-1.10344	
3.10000	1.17524	1.17853	-0.91206	-0.90998	
3.20000	1.23998	1.24167	-0.74630	-0.74594	-0.00097
3.30000	1.28439	1.28433	-0.60779	-0.60933	0.00116
3.40000	1.31034	1.30899	-0.49435	-0.49730	0.00269
3.50000	1.32025	1.31842	-0.40324	-0.40674	0.00330
3.60000	1.31671	1.31523	-0.33154	-0.33469	0.00300
3.70000	1.30230	1.30171	-0.27638	-0.27856	0.00205
3.80000	1.27938	1.27978	-0.23513	-0.23617	0.00089
3.90000	1.25001	1.25111	-0.20552	-0.20566	-0.00004
4.00000	1.21597	1.21722	-0.18561	-0.18535	-0.00045
4.10000	1.17877	1.17963	-0.17374	-0.17363	-0.00025
4.20000	1.13973	1.13987	-0.16851	-0.16887	0.00037
4.30000	1.10007	1.09947	-0.16862	-0.16949	0.00106

TABLE 10 (CONTINUED)

COMPARISON OF HELIUM PROPERTIES

T= 1.40 °K RHO=0.0218 ATOMS/Å^3

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K DIFFERENCE
4.40000	1.06090	1.05986	-0.17288	-0.17399	0.00146
4.50000	1.02332	1.02229	-0.18009	-0.18104	0.00132
4.60000	0.98837	0.98777	-0.18911	-0.18952	0.00062
4.70000	0.95703	0.95706	-0.19880	-0.19849	-0.00038
4.80000	0.93013	0.93073	-0.20813	-0.20719	-0.00131
4.90000	0.90835	0.90923	-0.21617	-0.21493	-0.00181
5.00000	0.89214	0.89291	-0.22218	-0.22103	-0.00168
5.10000	0.88168	0.88203	-0.22562	-0.22489	-0.00103
5.20000	0.87690	0.87671	-0.22619	-0.22600	-0.00018
5.30000	0.87746	0.87686	-0.22382	-0.22405	0.00049
5.40000	0.88282	0.88209	-0.21861	-0.21899	0.00071
5.50000	0.89225	0.89171	-0.21086	-0.21107	0.00043
5.60000	0.90494	0.90480	-0.20097	-0.20080	-0.00018
5.70000	0.92000	0.92028	-0.18940	-0.18882	-0.00081
5.80000	0.93657	0.93712	-0.17664	-0.17580	-0.00118
5.90000	0.95382	0.95440	-0.16314	-0.16231	-0.00116
6.00000	0.97103	0.97140	-0.14935	-0.14877	-0.00080
6.10000	0.98757	0.98758	-0.13563	-0.13543	-0.00025
6.20000	1.00290	1.00259	-0.12230	-0.12245	0.00024
6.30000	1.01660	1.01613	-0.10961	-0.10997	0.00050
6.40000	1.02838	1.02794	-0.09778	-0.09812	0.00047
6.50000	1.03798	1.03776	-0.08698	-0.08712	0.00020

TABLE 10 (CONTINUED)

COMPARISON OF HELIUM PROPERTIES

T= 1.40 °K RHO=0.0218 ATOMS/Å^3

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K DIFFERENCE
6.60000	1.04529	1.04535	-0.07732	-0.07720	-0.00016
6.70000	1.05024	1.05053	-0.06891	-0.06857	-0.00045
6.80000	1.05285	1.05323	-0.06179	-0.06137	-0.00055
6.90000	1.05324	1.05354	-0.05597	-0.05564	-0.00043
7.00000	1.05156	1.05166	-0.05142	-0.05130	-0.00016
7.10000	1.04806	1.04794	-0.04805	-0.04817	0.00015
7.20000	1.04304	1.04276	-0.04576	-0.04604	0.00037
7.30000	1.03683	1.03651	-0.04439	-0.04470	0.00042
7.40000	1.02979	1.02957	-0.04377	-0.04399	0.00029
7.50000	1.02228	1.02224	-0.04373	-0.04377	0.00005

TABLE 10 (CONTINUED)

COMPARISON OF HELIUM PROPERTIES

T= 4.20 °K RHO=0.0189 ATOMS/Å³

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K DIFFERENCE
0.0	-1.01324	-2.26059	-5.67664	-6.94767	
0.10000	-0.98430	-2.17371	-5.63851	-6.85095	
0.20000	-0.90022	-1.92639	-5.52706	-6.57441	
0.30000	-0.76888	-1.55576	-5.35078	-6.15601	
0.40000	-0.60247	-1.11516	-5.12283	-5.65038	
0.50000	-0.41619	-0.66352	-4.85968	-5.11813	
0.60000	-0.22658	-0.25453	-4.57941	-4.61485	
0.70000	-0.04982	0.07207	-4.29991	-4.18229	
0.80000	0.09991	0.29523	-4.03712	-3.84352	
0.90000	0.21188	0.41289	-3.80361	-3.60251	
1.00000	0.27971	0.43839	-3.60748	-3.44765	
1.10000	0.30192	0.39458	-3.45186	-3.35765	
1.20000	0.28180	0.30743	-3.33498	-3.30789	
1.30000	0.22688	0.20077	-3.25065	-3.27571	
1.40000	0.14787	0.09313	-3.18931	-3.24359	
1.50000	0.05744	-0.00308	-3.13933	-3.20000	
1.60000	-0.03123	-0.08072	-3.08838	-3.13857	
1.70000	-0.10583	-0.13600	-3.02491	-3.05621	
1.80000	-0.15606	-0.16667	-2.93927	-2.95130	
1.90000	-0.17455	-0.17086	-2.82469	-2.82256	
2.00000	-0.15734	-0.14678	-2.67772	-2.66875	
2.10000	-0.10396	-0.09325	-2.49843	-2.48921	

TABLE 10 (CONTINUED)

COMPARISON OF HELIUM PROPERTIES

T= 4.20 ^{0}K RHO=0.0189 ATOMS/Å^{3}

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K DIFFERENCE
2.20000	-0.01719	-0.01050	-2.29003	-2.28465	
2.30000	0.09754	0.09903	-2.05838	-2.05796	
2.40000	0.23296	0.23045	-1.81114	-1.81445	
2.50000	0.38082	0.37670	-1.55688	-1.56152	
2.60000	0.53278	0.52942	-1.30417	-1.30782	
2.70000	0.68116	0.68006	-1.06087	-1.06209	
2.80000	0.81955	0.82101	-0.83347	-0.83204	
2.90000	0.94313	0.94643	-0.62679	-0.62352	
3.00000	1.04879	1.05267	-0.44381	-0.44004	
3.10000	1.13511	1.13833	-0.28580	-0.28284	
3.20000	1.20207	1.20381	-0.15253	-0.15124	-0.00468
3.30000	1.25074	1.25083	-0.04267	-0.04323	0.00179
3.40000	1.28288	1.28171	0.04583	0.04386	0.00655
3.50000	1.30060	1.29892	0.11539	0.11280	0.00866
3.60000	1.30607	1.30464	0.16843	0.16605	0.00809
3.70000	1.30130	1.30064	0.20720	0.20565	0.00557
3.80000	1.28802	1.28828	0.23364	0.23311	0.00230
3.90000	1.26769	1.26864	0.24936	0.24966	-0.00049
4.00000	1.24156	1.24271	0.25568	0.25637	-0.00193
4.10000	1.21071	1.21155	0.25377	0.25435	-0.00175
4.20000	1.17619	1.17639	0.24471	0.24483	-0.00035
4.30000	1.13910	1.13862	0.22962	0.22922	0.00141

TABLE 10 (CONTINUED)

COMPARISON OF HELIUM PROPERTIES

T= 4.20 °K RHO=0.0189 ATOMS/$Å^3$

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K DIFFERENCE
4.40000	1.10062	1.09970	0.20971	0.20900	0.00253
4.50000	1.06203	1.06109	0.18629	0.18564	0.00234
4.60000	1.02470	1.02410	0.16077	0.16053	0.00073
4.70000	0.98994	0.98990	0.13458	0.13493	-0.00176
4.80000	0.95898	0.95947	0.10905	0.10994	-0.00414
4.90000	0.93284	0.93361	0.08540	0.08657	-0.00545
5.00000	0.91228	0.91298	0.06457	0.06567	-0.00519
5.10000	0.89770	0.89805	0.04724	0.04797	-0.00353
5.20000	0.88918	0.88906	0.03374	0.03400	-0.00128
5.30000	0.88644	0.88595	0.02414	0.02401	0.00056
5.40000	0.88894	0.88831	0.01819	0.01793	0.00123
5.50000	0.89592	0.89543	0.01549	0.01536	0.00060
5.60000	0.90648	0.90633	0.01549	0.01568	-0.00090
5.70000	0.91970	0.91992	0.01758	0.01811	-0.00248
5.80000	0.93466	0.93512	0.02117	0.02192	-0.00343
5.90000	0.95052	0.95101	0.02573	0.02649	-0.00336
6.00000	0.96656	0.96688	0.03083	0.03137	-0.00238
6.10000	0.98219	0.98222	0.03610	0.03631	-0.00094
6.20000	0.99691	0.99668	0.04129	0.04119	0.00038
6.30000	1.01037	1.01000	0.04619	0.04591	0.00113
6.40000	1.02228	1.02193	0.05065	0.05037	0.00116
6.50000	1.03241	1.03223	0.05456	0.05441	0.00060

TABLE 10 (CONTINUED)

COMPARISON OF HELIUM PROPERTIES

T= 4.20 °K RHO=0.0189 ATOMS/$Å^3$

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K DIFFERENCE
6.60000	1.04061	1.04065	0.05779	0.05784	-0.00020
6.70000	1.04677	1.04699	0.06024	0.06045	-0.00085
6.80000	1.05083	1.05111	0.06180	0.06207	-0.00107
6.90000	1.05277	1.05299	0.06240	0.06261	-0.00083
7.00000	1.05264	1.05272	0.06198	0.06204	-0.00025
7.10000	1.05057	1.05048	0.06052	0.06042	0.00040
7.20000	1.04675	1.04654	0.05806	0.05785	0.00085
7.30000	1.04143	1.04121	0.05470	0.05446	0.00094
7.40000	1.03494	1.03478	0.05056	0.05040	0.00066
7.50000	1.02762	1.02759	0.04583	0.04579	0.00015

TABLE 11

COMPARISON OF ARGON PROPERTIES

S	T=127.00 ^{0}K RHO=1.1350 GM/CC		T=127.00 ^{0}K RHO=1.0190 GM/CC		T=127.00 ^{0}K RHO=1.1160 GM/CC	
Å^{-1}	STRUCTURE FACTOR	CORRELATION INTENSITY	STRUCTURE FACTOR	CORRELATION INTENSITY	STRUCTURE FACTOR	CORRELATION INTENSITY
0.0	-0.78000	0.0	-0.75000	0.0	-0.77000	0.0
0.07720	-0.78258	-0.00015	-0.75200	-0.00015	-0.77347	-0.00014
0.15430	-0.78971	-0.00056	-0.75800	-0.00056	-0.78293	-0.00054
0.23150	-0.79988	-0.00118	-0.76699	-0.00119	-0.79604	-0.00115
0.30860	-0.81118	-0.00196	-0.77930	-0.00198	-0.81011	-0.00190
0.38570	-0.82187	-0.00284	-0.78971	-0.00287	-0.82287	-0.00276
0.46290	-0.83051	-0.00378	-0.80132	-0.00381	-0.83264	-0.00367
0.54000	-0.83772	-0.00472	-0.81258	-0.00476	-0.84045	-0.00458
0.61710	-0.84297	-0.00560	-0.82177	-0.00565	-0.84598	-0.00544
0.69420	-0.84543	-0.00638	-0.82792	-0.00644	-0.84831	-0.00620
0.77130	-0.84429	-0.00702	-0.83000	-0.00708	-0.84641	-0.00682
0.84830	-0.83858	-0.00746	-0.82685	-0.00753	-0.83927	-0.00725
0.92540	-0.82722	-0.00768	-0.81718	-0.00774	-0.82582	-0.00746
1.00240	-0.80918	-0.00761	-0.79969	-0.00768	-0.80476	-0.00740
1.07940	-0.78317	-0.00723	-0.77291	-0.00730	-0.77481	-0.00703
1.15640	-0.74799	-0.00649	-0.73524	-0.00655	-0.73435	-0.00631
1.23340	-0.70211	-0.00535	-0.68488	-0.00540	-0.68181	-0.00520
1.31040	-0.64418	-0.00377	-0.62057	-0.00381	-0.61750	-0.00367
1.38730	-0.56855	-0.00183	-0.53975	-0.00185	-0.54372	-0.00178
1.46420	-0.46056	0.00035	-0.42985	0.00035	-0.44153	0.00034
1.54110	-0.30392	0.00265	-0.27636	0.00267	-0.28985	0.00257
1.61790	-0.08117	0.00492	-0.06387	0.00496	-0.06519	0.00478

TABLE 11 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

S	T=127.00 °K RHO=1.1350 GM/CC		T=127.00 °K RHO=1.0190 GM/CC		T=127.00 °K RHO=1.1160 GM/CC	
$Å^{-1}$	STRUCTURE FACTOR	CORRELATION INTENSITY	STRUCTURE FACTOR	CORRELATION INTENSITY	STRUCTURE FACTOR	CORRELATION INTENSITY
1.69470	0.22705	0.00705	0.22469	0.00711	0.02585	0.00685
1.77150	0.52917	0.00891	0.50070	0.00899	0.56516	0.00866
1.84820	0.75144	0.01037	0.69682	0.01046	0.77356	0.01008
1.92490	0.86147	0.01131	0.78822	0.01141	0.86088	0.01099
2.00160	0.82499	0.01171	0.74750	0.01182	0.80312	0.01138
2.07830	0.60717	0.01165	0.54745	0.01175	0.57724	0.01132
2.15490	0.36853	0.01119	0.33328	0.01129	0.34625	0.01087
2.23140	0.15617	0.01041	0.16337	0.01050	0.17064	0.01012
2.30790	0.02801	0.00940	0.03276	0.00948	0.04083	0.00913
2.38440	-0.07955	0.00822	-0.06400	0.00829	-0.05453	0.00799
2.46080	-0.15047	0.00696	-0.13220	0.00702	-0.12820	0.00676
2.53720	-0.18943	0.00568	-0.18190	0.00573	-0.19231	0.00551
2.61350	-0.21299	0.00443	-0.21716	0.00447	-0.23943	0.00430
2.68980	-0.21242	0.00321	-0.23890	0.00324	-0.26619	0.00312
2.76600	-0.22375	0.00200	-0.24730	0.00202	-0.27352	0.00195
2.84220	-0.21247	0.00080	-0.24232	0.00081	-0.26318	0.00078
2.91830	-0.19144	-0.00040	-0.22401	-0.00040	-0.23659	-0.00039
2.99440	-0.16126	-0.00162	-0.19251	-0.00163	-0.19542	-0.00157
3.07040	-0.12334	-0.00286	-0.14806	-0.00289	-0.14233	-0.00278
3.14630	-0.07921	-0.00414	-0.09113	-0.00418	-0.07975	-0.00402
3.22220	-0.03045	-0.00545	-0.02245	-0.00550	-0.01048	-0.00530
3.29810	0.01472	-0.00674	0.04034	-0.00680	0.04917	-0.00655

TABLE 11 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

S	T=127.00 ^{0}K RHO=1.1350 GM/CC		T=127.00 ^{0}K RHO=1.0190 GM/CC		T=127.00 ^{0}K RHO=1.1160 GM/CC	
Å^{-1}	STRUCTURE FACTOR	CORRELATION INTENSITY	STRUCTURE FACTOR	CORRELATION INTENSITY	STRUCTURE FACTOR	CORRELATION INTENSITY
3.37380	0.05248	-0.00796	0.08983	-0.00803	0.09403	-0.00773
3.44950	0.08301	-0.00905	0.12645	-0.00913	0.12455	-0.00879
3.52520	0.10567	-0.00994	0.15082	-0.01003	0.14132	-0.00966
3.60070	0.12011	-0.01059	0.16363	-0.01068	0.14613	-0.01029
3.67620	0.12596	-0.01094	0.16614	-0.01103	0.13966	-0.01063
3.75170	0.12294	-0.01093	0.15873	-0.01102	0.12404	-0.01061
3.82700	0.11053	-0.01051	0.14278	-0.01060	0.10051	-0.01021
3.90230	0.08806	-0.00972	0.12005	-0.00981	0.07138	-0.00944
3.97750	0.05736	-0.00863	0.09216	-0.00871	0.03863	-0.00839
4.05260	0.01930	-0.00732	0.06031	-0.00738	0.00574	-0.00711
4.12770	-0.01320	-0.00585	0.02669	-0.00590	-0.02214	-0.00568
4.20270	-0.03929	-0.00430	-0.00632	-0.00433	-0.04416	-0.00417
4.27760	-0.05924	-0.00273	-0.03694	-0.00276	-0.06088	-0.00266
4.35240	-0.07328	-0.00123	-0.06243	-0.00124	-0.07224	-0.00120
4.42710	-0.08154	0.00014	-0.07985	0.00014	-0.07908	0.00014
4.50180	-0.08494	0.00134	-0.08681	0.00136	-0.08153	0.00131
4.57640	-0.08364	0.00237	-0.08552	0.00239	-0.07994	0.00230
4.65080	-0.07819	0.00320	-0.08160	0.00323	-0.07478	0.00311
4.72520	-0.06916	0.00385	-0.07551	0.00388	-0.06630	0.00374
4.79950	-0.05698	0.00430	-0.06692	0.00434	-0.05559	0.00418
4.87370	-0.04279	0.00456	-0.05636	0.00460	-0.04295	0.00443
4.94780	-0.02712	0.00461	-0.04431	0.00465	-0.02881	0.00448

TABLE 11 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

	T=127.00 °K RHO=1.1350 GM/CC		T=127.00 °K RHO=1.0190 GM/CC		T=127.00 °K RHO=1.1160 GM/CC	
S Å^{-1}	STRUCTURE FACTOR	CORRELATION INTENSITY	STRUCTURE FACTOR	CORRELATION INTENSITY	STRUCTURE FACTOR	CORRELATION INTENSITY
5.02190	-0.01056	0.00445	-0.03054	0.00449	-0.01440	0.00433
5.09580	0.00547	0.00409	-0.01570	0.00413	-0.00000	0.00398
5.16960	0.02067	0.00355	-0.00000	0.00358		
5.24340	0.03336	0.00287				
5.31700	0.04303	0.00207				
5.39050	0.04826	0.00120				
5.46390	0.04761	0.00029				
5.53730	0.04116	-0.00063				
5.61050	0.03383	-0.00152				
5.68360	0.02661	-0.00234				
5.75660	0.01960	-0.00309				
5.82950	0.01278	-0.00375				
5.90230	0.00638	-0.00432				
5.97490	-0.00000	-0.00479				

TABLE 11 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

S	T=143.00 °K RHO=0.9100 GM/CC		T=133.00 °K RHO=1.0540 GM/CC		T= RHO=	
Å^{-1}	STRUCTURE FACTOR	CORRELATION INTENSITY	STRUCTURE FACTOR	CORRELATION INTENSITY	STRUCTURE FACTOR	CORRELATION INTENSITY
0.0	0.29000	0.0	-0.60000	0.0		
0.07720	0.13990	-0.00006	-0.61444	-0.00014		
0.15430	-0.14507	-0.00021	-0.65070	-0.00054		
0.23150	-0.37940	-0.00045	-0.69443	-0.00114		
0.30860	-0.53130	-0.00074	-0.73434	-0.00189		
0.38570	-0.62127	-0.00107	-0.76504	-0.00274		
0.46290	-0.66760	-0.00143	-0.78460	-0.00365		
0.54000	-0.69530	-0.00178	-0.79819	-0.00455		
0.61710	-0.71980	-0.00211	-0.80953	-0.00541		
0.69420	-0.73907	-0.00241	-0.81734	-0.00616		
0.77130	-0.75087	-0.00265	-0.82070	-0.00677		
0.84830	-0.75302	-0.00282	-0.81763	-0.00720		
0.92540	-0.74309	-0.00290	-0.80726	-0.00741		
1.00240	-0.71810	-0.00287	-0.78793	-0.00735		
1.07940	-0.67860	-0.00273	-0.75782	-0.00698		
1.15640	-0.62920	-0.00245	-0.71509	-0.00627		
1.23340	-0.56681	-0.00202	-0.65767	-0.00516		
1.31040	-0.48800	-0.00142	-0.58405	-0.00364		
1.38730	-0.38950	-0.00069	-0.49323	-0.00177		
1.46420	-0.26706	0.00013	-0.37641	0.00034		
1.54110	-0.11667	0.00100	-0.22421	0.00255		
1.61790	0.06654	0.00186	-0.02590	0.00475		

TABLE 11 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

S Å^{-1}	STRUCTURE FACTOR	CORRELATION INTENSITY	STRUCTURE FACTOR	CORRELATION INTENSITY	STRUCTURE FACTOR	CORRELATION INTENSITY
	T=143.00 °K RHO=0.9100 GM/CC		T=133.00 °K RHO=1.0540 GM/CC		T= RHO=	
1.69470	0.28797	0.00266	0.23076	0.00680		
1.77150	0.45752	0.00336	0.47914	0.00860		
1.84820	0.53872	0.00391	0.66224	0.01001		
1.92490	0.54459	0.00427	0.75160	0.01092		
2.00160	0.49067	0.00442	0.71580	0.01131		
2.07830	0.39290	0.00439	0.52326	0.01124		
2.15490	0.26993	0.00422	0.31829	0.01080		
2.23140	0.14172	0.00393	0.15885	0.01005		
2.30790	0.03174	0.00355	0.03977	0.00907		
2.38440	-0.04202	0.00310	-0.04591	0.00793		
2.46080	-0.09869	0.00262	-0.10595	0.00671		
2.53720	-0.14092	0.00214	-0.14816	0.00548		
2.61350	-0.17013	0.00167	-0.17994	0.00428		
2.68980	-0.18649	0.00121	-0.20129	0.00310		
2.76600	-0.19080	0.00076	-0.21180	0.00193		
2.84220	-0.18403	0.00030	-0.21106	0.00078		
2.91830	-0.16728	-0.00015	-0.19867	-0.00039		
2.99440	-0.14172	-0.00061	-0.17426	-0.00156		
3.07040	-0.11053	-0.00108	-0.13751	-0.00276		
3.14630	-0.07709	-0.00156	-0.08821	-0.00400		
3.22220	-0.04190	-0.00206	-0.02640	-0.00526		
3.29810	-0.00647	-0.00254	0.03003	-0.00651		

TABLE 11 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

S	T=143.00 °K RHO=0.9100 GM/CC		T=133.00 °K RHO=1.0540 GM/CC		T= RHO=	
$Å^{-1}$	STRUCTURE FACTOR	CORRELATION INTENSITY	STRUCTURE FACTOR	CORRELATION INTENSITY	STRUCTURE FACTOR	CORRELATION INTENSITY
3.37380	0.02836	-0.00300	0.07350	-0.00768		
3.44950	0.06160	-0.00341	0.10455	-0.00873		
3.52520	0.09147	-0.00375	0.12395	-0.00959		
3.60070	0.11702	-0.00400	0.13256	-0.01022		
3.67620	0.13619	-0.00413	0.13179	-0.01056		
3.75170	0.14780	-0.00412	0.12224	-0.01054		
3.82700	0.14933	-0.00396	0.10544	-0.01014		
3.90230	0.13947	-0.00367	0.08336	-0.00938		
3.97750	0.11620	-0.00326	0.05784	-0.00833		
4.05260	0.08115	-0.00276	0.03031	-0.00706		
4.12770	0.04929	-0.00221	0.00344	-0.00564		
4.20270	0.02163	-0.00162	-0.02088	-0.00415		
4.27760	-0.00212	-0.00103	-0.04013	-0.00264		
4.35240	-0.02160	-0.00046	-0.05436	-0.00119		
4.42710	-0.03736	0.00005	-0.06405	0.00014		
4.50180	-0.04913	0.00051	-0.06905	0.00130		
4.57640	-0.05733	0.00089	-0.06994	0.00228		
4.65080	-0.06216	0.00121	-0.06710	0.00309		
4.72520	-0.06386	0.00145	-0.06096	0.00371		
4.79950	-0.06276	0.00162	-0.05206	0.00415		
4.87370	-0.05915	0.00172	-0.04089	0.00440		
4.94780	-0.05344	0.00174	-0.02811	0.00445		

TABLE 11 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

S $Å^{-1}$	T=143.00 °K RHO=0.9100 GM/CC STRUCTURE FACTOR	 CORRELATION INTENSITY	T=133.00 °K RHO=1.0540 GM/CC STRUCTURE FACTOR	 CORRELATION INTENSITY	T= RHO= STRUCTURE FACTOR	 CORRELATION INTENSITY
5.02190	-0.04598	0.00168	-0.01404	0.00430		
5.09580	-0.03731	0.00154	-0.00000	0.00395		
5.16960	-0.02782	0.00134				
5.24340	-0.01786	0.00108				
5.31700	-0.00845	0.00078				
5.39050	-0.00000	0.00045				

TABLE 12

COMPARISON OF ARGON PROPERTIES

T=127.00 °K RHO=1.1350 GM/CC

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K	U(R)/K CORRELATED
0.0	0.63528	0.45522	-10.71703	-11.23292		
0.10000	0.60180	0.42783	-10.70204	-11.21259		
0.20000	0.51005	0.35355	-10.65122	-11.14643		
0.30000	0.38378	0.25383	-10.54904	-11.02081		
0.40000	0.25533	0.15772	-10.37571	-10.81862		
0.50000	0.15680	0.09371	-10.11449	-10.52600		
0.60000	0.11134	0.08169	-9.75867	-10.13875		
0.70000	0.12691	0.12717	-9.31608	-9.66648		
0.80000	0.19412	0.21931	-8.80987	-9.13324		
0.90000	0.28686	0.33346	-8.27489	-8.57408		
1.00000	0.37894	0.43747	-7.75075	-8.02848		
1.10000	0.43286	0.50004	-7.27316	-7.53204		
1.20000	0.42847	0.49905	-6.86592	-7.10884		
1.30000	0.35901	0.42747	-6.53573	-6.76626		
1.40000	0.23499	0.29538	-6.27118	-6.49384		
1.50000	0.08142	0.12755	-6.04635	-6.26642		
1.60000	-0.06890	-0.04284	-5.82807	-6.05094		
1.70000	-0.18415	-0.18264	-5.58485	-5.81501		
1.80000	-0.24191	-0.26700	-5.29536	-5.53521		
1.90000	-0.23507	-0.28548	-4.95401	-5.20288		
2.00000	-0.17342	-0.24425	-4.57223	-4.82591		
2.10000	-0.08074	-0.16378	-4.17513	-4.42624		

TABLE 12 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

T=127.00 °K RHO=1.1350 GM/CC

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K	U(R)/K CORRELATED
2.20000	0.01206	-0.07286	-3.79450	-4.03348		
2.30000	0.07577	-0.00029	-3.45974	-3.67657		
2.40000	0.09134	0.03340	-3.18950	-3.37554		
2.50000	0.05583	0.02204	-2.98582	-3.13558		
2.60000	-0.01593	-0.02382	-2.83275	-2.94488		
2.70000	-0.09429	-0.07899	-2.69943	-2.77700		
2.80000	-0.14173	-0.10965	-2.54729	-2.59700		
2.90000	-0.12197	-0.08171	-2.33925	-2.36999		
3.00000	-0.00915	0.03042	-2.04890	-2.06984		
3.10000	0.20541	0.23695	-1.66730	-1.68611		
3.20000	0.51024	0.52932	-1.20583	-1.22735	154.04020	152.34701
3.30000	0.87539	0.88107	-0.69447	-0.72011	74.17736	75.86445
3.40000	1.25823	1.25278	-0.17593	-0.20396	16.62068	19.15635
3.50000	1.61188	1.59977	0.30283	0.27629	-26.42873	-24.07867
3.60000	1.89430	1.88083	0.69973	0.67935	-58.55459	-56.91648
3.70000	2.07603	2.06590	0.98530	0.97515	-81.73867	-81.11471
3.80000	2.14487	2.14110	1.14743	1.14986	-97.23680	-97.80546
3.90000	2.10672	2.11014	1.19218	1.20738	-105.97743	-107.82952
4.00000	1.98267	1.99205	1.14092	1.16702	-108.80364	-111.95073
4.10000	1.80337	1.81607	1.02472	1.05846	-106.66085	-111.03227
4.20000	1.60212	1.61499	0.87740	0.91509	-100.74940	-106.19103
4.30000	1.40832	1.41868	0.72904	0.76747	-92.59843	-98.88952

TABLE 12 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

T=127.00 ^{0}K RHO=1.1350 GM/CC

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K	U(R)/K CORRELATED
4.40000	1.24279	1.24906	0.60117	0.63833	-83.96245	-90.86649
4.50000	1.11558	1.11756	0.50457	0.53987	-76.45697	-83.80269
4.60000	1.02653	1.02521	0.43974	0.47386	-71.02768	-78.77633
4.70000	0.96794	0.96499	0.39949	0.43387	-67.59733	-75.83657
4.80000	0.92844	0.92558	0.37280	0.40897	-65.20118	-74.05910
4.90000	0.89682	0.89528	0.34867	0.38767	-62.52295	-72.06207
5.00000	0.86511	0.86529	0.31916	0.36117	-58.46271	-68.61224
5.10000	0.82994	0.83143	0.28096	0.32526	-52.48752	-63.02782
5.20000	0.79255	0.79436	0.23534	0.28056	-44.74398	-55.33369
5.30000	0.75732	0.75834	0.18688	0.23137	-35.98916	-46.22683
5.40000	0.72978	0.72919	0.14145	0.18376	-27.36274	-36.87527
5.50000	0.71459	0.71216	0.10421	0.14339	-20.01894	-28.55365
5.60000	0.71415	0.71029	0.07817	0.11391	-14.72232	-22.19976
5.70000	0.72805	0.72368	0.06357	0.09612	-11.60434	-18.09898
5.80000	0.75350	0.74974	0.05825	0.08813	-10.21850	-15.88202
5.90000	0.78640	0.78416	0.05856	0.08629	-9.82737	-14.80624
6.00000	0.82252	0.82225	0.06062	0.08646	-9.72209	-14.10942
6.10000	0.85868	0.86023	0.06142	0.08524	-9.42573	-13.25294
6.20000	0.89325	0.89596	0.05949	0.08083	-8.75290	-12.00732
6.30000	0.92617	0.92910	0.05493	0.07318	-7.76500	-10.41924
6.40000	0.95841	0.96063	0.04903	0.06369	-6.66975	-8.71255
6.50000	0.99113	0.99202	0.04353	0.05441	-5.70452	-7.16449

TABLE 12 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

T=127.00 ^{0}K RHO=1.1350 GM/CC

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K	U(R)/K CORRELATED
6.60000	1.02490	1.02434	0.03986	0.04721	-5.03752	-5.99182
6.70000	1.05919	1.05751	0.03859	0.04305	-4.71340	-5.27796
6.80000	1.09226	1.09013	0.03930	0.04174	-4.65313	-4.95849
6.90000	1.12156	1.11973	0.04072	0.04204	-4.69662	-4.85960
7.00000	1.14428	1.14336	0.04126	0.04210	-4.66348	-4.76496
7.10000	1.15818	1.15840	0.03951	0.04018	-4.40820	-4.48301
7.20000	1.16209	1.16331	0.03476	0.03514	-3.85644	-3.89573
7.30000	1.15623	1.15800	0.02716	0.02688	-3.01889	-2.98260
7.40000	1.14217	1.14387	0.01771	0.01628	-1.98468	-1.82017
7.50000	1.12235	1.12344	0.00790	0.00495	-0.89743	-0.56032
7.60000	1.09957	1.09977	-0.00071	-0.00529	0.08164	0.60932
7.70000	1.07638	1.07572	-0.00694	-0.01292	0.81653	1.51611
7.80000	1.05462	1.05341	-0.01030	-0.01716	1.23440	2.05233
7.90000	1.03521	1.03393	-0.01103	-0.01813	1.34607	2.20809
8.00000	1.01823	1.01736	-0.01000	-0.01675	1.24099	2.07410
8.10000	1.00319	1.00303	-0.00839	-0.01441	1.05777	1.81174
8.20000	0.98936	0.98994	-0.00736	-0.01256	0.94106	1.60151
8.30000	0.97618	0.97728	-0.00772	-0.01230	0.99986	1.58883
8.40000	0.96346	0.96469	-0.00976	-0.01411	1.27995	1.84440
8.50000	0.95148	0.95240	-0.01325	-0.01778	1.75667	2.34941

TABLE 12 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

T=127.00 °K RHO=1.0190 GM/CC

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K	U(R)/K CORRELATED
0.0	-1.05254	-1.16309	-10.00000	-10.00000		
0.10000	-0.98624	-1.09556	-10.00000	-10.00000		
0.20000	-0.79851	-0.90383	-10.00000	-10.00000		
0.30000	-0.52078	-0.61863	-11.76514	-12.16622		
0.40000	-0.19905	-0.28506	-11.09243	-11.49058		
0.50000	0.11444	0.04531	-10.35989	-10.75032		
0.60000	0.37053	0.32344	-9.63627	-10.01279		
0.70000	0.53182	0.51116	-8.97864	-9.33461		
0.80000	0.57897	0.58734	-8.42440	-8.75400		
0.90000	0.51355	0.55093	-7.98712	-8.28652		
1.00000	0.35703	0.42014	-7.65675	-7.92509		
1.10000	0.14599	0.22829	-7.40404	-7.64389		
1.20000	-0.07523	0.01693	-7.18815	-7.40530		
1.30000	-0.26316	-0.17221	-6.96588	-7.16857		
1.40000	-0.38346	-0.30508	-6.70077	-6.89838		
1.50000	-0.41706	-0.36129	-6.37032	-6.57181		
1.60000	-0.36328	-0.33739	-5.97001	-6.18236		
1.70000	-0.23929	-0.24666	-5.51356	-5.74052		
1.80000	-0.07609	-0.11568	-5.02941	-5.27082		
1.90000	0.08810	0.02152	-4.55434	-4.80609		
2.00000	0.21572	0.13079	-4.12554	-4.38023		
2.10000	0.27751	0.18491	-3.77271	-4.02084		

TABLE 12 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

T=127.00 °K RHO=1.0190 GM/CC

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K	U(R)/K CORRELATED
2.20000	0.25848	0.16928	-3.51173	-3.74329		
2.30000	0.16102	0.08504	-3.34123	-3.54722		
2.40000	0.00468	-0.05087	-3.24240	-3.41624		
2.50000	-0.17729	-0.20866	-3.18232	-3.32075		
2.60000	-0.34389	-0.35109	-3.11989	-3.22323		
2.70000	-0.45384	-0.44024	-3.01330	-3.08518		
2.80000	-0.47290	-0.44436	-2.82760	-2.87408		
2.90000	-0.37998	-0.34365	-2.54097	-2.56939		
3.00000	-0.17083	-0.13384	-2.14861	-2.16631		
3.10000	0.14124	0.17295	-1.66361	-1.67679		
3.20000	0.52754	0.55003	-1.11477	-1.12767	144.22575	141.63045
3.30000	0.94875	0.96047	-0.54181	-0.55636	57.37403	58.03326
3.40000	1.36114	1.36281	0.01095	-0.00496	-1.02569	0.46171
3.50000	1.72323	1.71737	0.50146	0.48617	-43.67563	-42.26635
3.60000	2.00171	1.99185	0.89602	0.88427	-75.37831	-74.53407
3.70000	2.17565	2.16553	1.17359	1.16840	-98.45875	-98.49354
3.80000	2.23855	2.23130	1.32791	1.33165	-114.22810	-115.35842
3.90000	2.19785	2.19549	1.36702	1.38090	-123.54679	-125.91653
4.00000	2.07245	2.07562	1.31066	1.33451	-127.10452	-130.79198
4.10000	1.88865	1.89670	1.18612	1.21851	-125.59485	-130.61299
4.20000	1.67548	1.68676	1.02339	1.06202	-119.84646	-126.14026
4.30000	1.46020	1.47256	0.85054	0.89274	-110.92665	-118.36986

TABLE 12 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

T=127.00 ^{0}K RHO=1.0190 GM/CC

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K	U(R)/K CORRELATED
4.40000	1.26468	1.27599	0.69008	0.73335	-100.19109	-108.58798
4.50000	1.10327	1.11186	0.55673	0.59917	-89.20751	-98.31193
4.60000	0.98214	0.98708	0.45685	0.49744	-79.47372	-89.03668
4.70000	0.90015	0.90135	0.38940	0.42803	-71.96832	-81.80328
4.80000	0.85076	0.84884	0.34795	0.38524	-66.79274	-76.81554
4.90000	0.82451	0.82057	0.32328	0.36026	-63.21066	-73.41779
5.00000	0.81151	0.80682	0.30589	0.34366	-60.08613	-70.48774
5.10000	0.80346	0.79917	0.28813	0.32748	-56.40385	-66.96139
5.20000	0.79500	0.79185	0.26540	0.30659	-51.59122	-62.18957
5.30000	0.78403	0.78233	0.23649	0.27914	-45.59509	-56.04666
5.40000	0.77139	0.77099	0.20307	0.24625	-38.79968	-48.86624
5.50000	0.75992	0.76034	0.16864	0.21104	-31.86762	-41.29080
5.60000	0.75322	0.75385	0.13723	0.17743	-25.54269	-34.08046
5.70000	0.75451	0.75479	0.11217	0.14889	-20.43986	-27.90585
5.80000	0.76576	0.76535	0.09525	0.12762	-16.86996	-23.16669
5.90000	0.78727	0.78610	0.08640	0.11400	-14.76421	-19.89759
6.00000	0.81768	0.81596	0.08381	0.10672	-13.73279	-17.80121
6.10000	0.85440	0.85252	0.08449	0.10320	-13.22408	-16.38758
6.20000	0.89421	0.89265	0.08513	0.10036	-12.70493	-15.14714
6.30000	0.93399	0.93312	0.08282	0.09533	-11.79231	-13.68701
6.40000	0.97121	0.97123	0.07573	0.08617	-10.31022	-11.79868
6.50000	1.00427	1.00516	0.06340	0.07217	-8.28194	-9.46222

TABLE 12 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

T=127.00 °K RHO=1.0190 GM/CC

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K	U(R)/K CORRELATED
6.60000	1.03257	1.03408	0.04673	0.05398	-5.88178	-6.80888
6.70000	1.05628	1.05803	0.02765	0.03332	-3.36894	-4.06331
6.80000	1.07606	1.07761	0.00861	0.01250	-1.02010	-1.48128
6.90000	1.09262	1.09360	-0.00802	-0.00610	0.92828	0.70647
7.00000	1.10643	1.10666	-0.02040	-0.02055	2.32027	2.33675
7.10000	1.11756	1.11703	-0.02761	-0.02975	3.09930	3.33790
7.20000	1.12564	1.12455	-0.02968	-0.03355	3.30558	3.73345
7.30000	1.13001	1.12868	-0.02752	-0.03271	3.05622	3.62785
7.40000	1.12993	1.12875	-0.02260	-0.02862	2.51500	3.17993
7.50000	1.12490	1.12417	-0.01659	-0.02299	1.85959	2.57116
7.60000	1.11478	1.11469	-0.01105	-0.01747	1.25223	1.97522
7.70000	1.09996	1.10054	-0.00711	-0.01337	0.81786	1.53342
7.80000	1.08134	1.08242	-0.00539	-0.01147	0.63165	1.33866
7.90000	1.06015	1.06146	-0.00600	-0.01201	0.71641	1.42890
8.00000	1.03781	1.03903	-0.00861	-0.01475	1.04929	1.79036
8.10000	1.01569	1.01654	-0.01268	-0.01914	1.57549	2.36888
8.20000	0.99495	0.99525	-0.01759	-0.02449	2.22572	3.08691
8.30000	0.97641	0.97612	-0.02281	-0.03014	2.93231	3.86175
8.40000	0.96055	0.95979	-0.02793	-0.03556	3.63995	4.62033
8.50000	0.94757	0.94656	-0.03270	-0.04039	4.30846	5.30711

TABLE 12 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

T=127.00 °K RHO=1.1160 GM/CC

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K	U(R)/K CORRELATED
0.0	-1.78147	-1.90049	-10.00000	-10.00000		
0.10000	-1.70365	-1.82063	-10.00000	-10.00000		
0.20000	-1.48102	-1.59180	-10.00000	-10.00000		
0.30000	-1.14448	-1.24468	-12.19649	-12.61851		
0.40000	-0.73988	-0.82492	-11.47821	-11.88928		
0.50000	-0.32064	-0.38606	-10.68122	-11.07671		
0.60000	0.06062	0.01877	-9.87395	-10.24900		
0.70000	0.36024	0.34471	-9.11624	-9.46642		
0.80000	0.54977	0.56150	-8.45179	-8.77394		
0.90000	0.61957	0.65714	-7.90359	-8.19646		
1.00000	0.57905	0.63843	-7.47294	-7.73776		
1.10000	0.45365	0.52833	-7.14213	-7.38267		
1.20000	0.27940	0.36088	-6.88001	-7.10226		
1.30000	0.09581	0.17455	-6.64932	-6.86077		
1.40000	-0.06126	0.00529	-6.41446	-6.62300		
1.50000	-0.16569	-0.11945	-6.14822	-6.36098		
1.60000	-0.20502	-0.18475	-5.83634	-6.05849		
1.70000	-0.18153	-0.18962	-5.47916	-5.71308		
1.80000	-0.11055	-0.14581	-5.09031	-5.33514		
1.90000	-0.01631	-0.07414	-4.69278	-4.94448		
2.00000	0.07368	0.00058	-4.31330	-4.56528		
2.10000	0.13468	0.05523	-3.97618	-4.22029		

TABLE 12 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

T=127.00 °K RHO=1.1160 GM/CC

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K	U(R)/K CORRELATED
2.20000	0.15003	0.07344	-3.69786	-3.92563		
2.30000	0.11461	0.04908	-3.48319	-3.68712		
2.40000	0.03610	-0.01230	-3.32407	-3.49869		
2.50000	-0.06640	-0.09443	-3.20071	-3.34333		
2.60000	-0.16589	-0.17336	-3.08519	-3.19611		
2.70000	-0.23246	-0.22200	-2.94658	-3.02885		
2.80000	-0.23885	-0.21523	-2.75662	-2.81537		
2.90000	-0.16553	-0.13467	-2.49500	-2.53648		
3.00000	-0.00436	0.02773	-2.15313	-2.18368		
3.10000	0.23977	0.26792	-1.73596	-1.76103		
3.20000	0.54943	0.57007	-1.26137	-1.28480	151.46585	149.83553
3.30000	0.89732	0.90884	-0.75749	-0.78121	77.72718	78.78396
3.40000	1.25042	1.25312	-0.25841	-0.28244	23.85770	25.81395
3.50000	1.57486	1.57065	0.20094	0.17812	-17.33510	-15.28707
3.60000	1.84083	1.83259	0.58984	0.57069	-49.05772	-47.38467
3.70000	2.02648	2.01742	0.88590	0.87307	-72.99508	-72.00701
3.80000	2.12048	2.11344	1.07767	1.07340	-90.13523	-90.05025
3.90000	2.12276	2.11969	1.16543	1.17101	-101.13355	-102.10143
4.00000	2.04350	2.04525	1.16014	1.17569	-106.51261	-108.62210
4.10000	1.90076	1.90700	1.08092	1.10543	-106.79327	-110.07349
4.20000	1.71716	1.72664	0.95161	0.98319	-102.59458	-107.01477
4.30000	1.51628	1.52722	0.79703	0.83332	-94.71768	-100.18735

TABLE 12 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

T=127.00 °K RHO=1.1160 GM/CC

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K	U(R)/K CORRELATED
4.40000	1.31949	1.32996	0.63961	0.67822	-84.21196	-90.58374
4.50000	1.14340	1.15179	0.49681	0.53578	-72.39602	-79.47712
4.60000	0.99860	1.00387	0.37978	0.41783	-60.77387	-68.35520
4.70000	0.88942	0.89124	0.29316	0.32982	-50.78639	-58.69268
4.80000	0.81475	0.81349	0.23598	0.27150	-43.43032	-51.57258
4.90000	0.76955	0.76608	0.20322	0.23835	-38.94155	-47.33275
5.00000	0.74668	0.74214	0.18777	0.22346	-36.78609	-45.49732
5.10000	0.73867	0.73418	0.18227	0.21934	-35.98803	-45.07081
5.20000	0.73916	0.73559	0.18055	0.21943	-35.56747	-44.99069
5.30000	0.74371	0.74151	0.17846	0.21908	-34.84686	-44.47488
5.40000	0.75004	0.74926	0.17412	0.21586	-33.54898	-43.15713
5.50000	0.75779	0.75812	0.16757	0.20939	-31.73798	-41.04988
5.60000	0.76789	0.76878	0.16004	0.20066	-29.68146	-38.41492
5.70000	0.78173	0.78259	0.15316	0.19134	-27.69398	-35.60613
5.80000	0.80049	0.80085	0.14822	0.18291	-26.00485	-32.92861
5.90000	0.82462	0.82424	0.14565	0.17621	-24.68215	-30.54631
6.00000	0.85366	0.85256	0.14492	0.17114	-23.67716	-28.45605
6.10000	0.88627	0.88470	0.14465	0.16675	-22.62911	-26.52369
6.20000	0.92060	0.91896	0.14306	0.16157	-21.44945	-24.55723
6.30000	0.95465	0.95336	0.13846	0.15406	-19.90094	-22.38386
6.40000	0.98670	0.98607	0.12970	0.14305	-17.89839	-19.90590
6.50000	1.01554	1.01573	0.11650	0.12813	-15.47422	-17.12540

TABLE 12 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

T=127.00 °K RHO=1.1160 GM/CC

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K	U(R)/K CORRELATED
6.60000	1.04065	1.04158	0.09950	0.10974	-12.76362	-14.13930
6.70000	1.06206	1.06349	0.08018	0.08911	-9.96939	-11.11343
6.80000	1.08018	1.08174	0.06048	0.06800	-7.31726	-8.24489
6.90000	1.09551	1.09683	0.04239	0.04832	-5.01148	-5.72160
7.00000	1.10837	1.10916	0.02757	0.03174	-3.19885	-3.68702
7.10000	1.11876	1.11885	0.01702	0.01935	-1.94704	-2.21603
7.20000	1.12626	1.12570	0.01094	0.01151	-1.24003	-1.30572
7.30000	1.13020	1.12917	0.00877	0.00781	-0.98933	-0.88130
7.40000	1.12977	1.12858	0.00936	0.00721	-1.05663	-0.81436
7.50000	1.12433	1.12329	0.01129	0.00835	-1.28192	-0.94813
7.60000	1.11360	1.11299	0.01317	0.00981	-1.51125	-1.12467
7.70000	1.09784	1.09781	0.01392	0.01040	-1.62014	-1.20908
7.80000	1.07788	1.07844	0.01290	0.00937	-1.52952	-1.10780
7.90000	1.05504	1.05603	0.01003	0.00646	-1.21288	-0.77874
8.00000	1.03092	1.03210	0.00561	0.00188	-0.69354	-0.23206
8.10000	1.00722	1.00831	0.00026	-0.00381	-0.03242	0.47877
8.20000	0.98544	0.98618	-0.00538	-0.00995	0.69156	1.27439
8.30000	0.96668	0.96692	-0.01074	-0.01590	1.40384	2.07159
8.40000	0.95159	0.95130	-0.01551	-0.02124	2.05329	2.80443
8.50000	0.94031	0.93960	-0.01961	-0.02578	2.62172	3.43791

TABLE 12 9(CONTINUED)

COMPARISON OF ARGON PROPERTIES

T=143.00 ^{0}K RHO=0.9100 GM/CC

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K	U(R)/K CORRELATED
0.0	-0.67960	-0.70504	-8.26625	-8.33264		
0.10000	-0.61411	-0.63999	-8.16074	-8.22842		
0.20000	-0.43009	-0.45698	-7.85920	-7.93038		
0.30000	-0.16232	-0.19009	-7.40388	-7.47973		
0.40000	0.13890	0.11141	-6.85650	-6.93670		
0.50000	0.41774	0.39267	-6.28709	-6.36978		
0.60000	0.62377	0.60396	-5.76152	-5.84354		
0.70000	0.72170	0.71013	-5.33019	-5.40769		
0.80000	0.69796	0.69714	-5.02007	-5.08929		
0.90000	0.56295	0.57420	-4.83146	-4.88954		
1.00000	0.34829	0.37134	-4.74008	-4.78571		
1.10000	0.10007	0.13282	-4.70376	-4.73754		
1.20000	-0.13082	-0.09212	-4.67242	-4.69683		
1.30000	-0.29900	-0.25930	-4.59903	-4.61810		
1.40000	-0.37366	-0.33834	-4.44958	-4.46811		
1.50000	-0.34442	-0.31844	-4.20979	-4.23257		
1.60000	-0.22295	-0.21002	-3.88757	-3.91844		
1.70000	-0.04002	-0.04204	-3.51070	-3.55190		
1.80000	0.16115	0.14447	-3.12040	-3.17216		
1.90000	0.33415	0.30514	-2.76232	-2.82285		
2.00000	0.43890	0.40159	-2.47670	-2.54251		
2.10000	0.45001	0.40936	-2.28982	-2.35637		

TABLE 12 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

T=143.00 °K RHO=0.9100 GM/CC

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K	U(R)/K CORRELATED
2.20000	0.36187	0.32301	-2.20847	-2.27097		
2.30000	0.18993	0.15734	-2.21837	-2.27258		
2.40000	-0.03222	-0.05539	-2.28683	-2.32974		
2.50000	-0.25927	-0.27154	-2.36902	-2.39922		
2.60000	-0.44266	-0.44433	-2.41642	-2.43422		
2.70000	-0.53953	-0.53239	-2.38586	-2.39305		
2.80000	-0.52039	-0.50729	-2.24735	-2.24677		
2.90000	-0.37420	-0.35840	-1.98925	-1.98417		
3.00000	-0.10983	-0.09444	-1.61994	-1.61346		
3.10000	0.24585	0.25842	-1.16590	-1.16044		
3.20000	0.65311	0.66143	-0.66662	-0.66365	100.59189	99.35999
3.30000	1.06625	1.06998	-0.16767	-0.16758	20.88517	20.80722
3.40000	1.44113	1.44090	0.28691	0.28465	-31.74642	-31.47256
3.50000	1.74184	1.73892	0.66134	0.65790	-68.28456	-67.97673
3.60000	1.94539	1.94136	0.93282	0.92965	-93.37513	-93.19912
3.70000	2.04386	2.04023	1.09372	1.09212	-109.53591	-109.58852
3.80000	2.04380	2.04169	1.15088	1.15179	-118.41438	-118.75140
3.90000	1.96333	1.96333	1.12271	1.12650	-121.30028	-121.94706
4.00000	1.82770	1.82981	1.03461	1.04109	-119.38783	-120.34297
4.10000	1.66433	1.66808	0.91402	0.92256	-113.92809	-115.16394
4.20000	1.49819	1.50282	0.78576	0.79546	-106.29689	-107.75995
4.30000	1.34846	1.35312	0.66869	0.67866	-97.94886	-99.56440

TABLE 12 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

T=143.00 °K RHO=0.9100 GM/CC

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K	U(R)/K CORRELATED
4.40000	1.22668	1.23062	0.57396	0.58348	-90.22136	-91.90735
4.50000	1.13663	1.13939	0.50505	0.51371	-84.02529	-85.71536
4.60000	1.07565	1.07705	0.45911	0.46685	-79.58705	-81.25274
4.70000	1.03678	1.03696	0.42930	0.43638	-76.44241	-78.09972
4.80000	1.01136	1.01065	0.40738	0.41421	-73.71891	-75.41431
4.90000	0.99124	0.99006	0.38594	0.39298	-70.53124	-72.31643
5.00000	0.97047	0.96921	0.35997	0.36759	-66.28077	-68.18969
5.10000	0.94605	0.94499	0.32756	0.33592	-60.77727	-62.81273
5.20000	0.91788	0.91714	0.28964	0.29869	-54.21699	-56.34735
5.30000	0.88809	0.88765	0.24913	0.25860	-47.08062	-49.24428
5.40000	0.85995	0.85969	0.20980	0.21928	-39.99309	-42.10888
5.50000	0.83685	0.83661	0.17509	0.18414	-33.56710	-35.54888
5.60000	0.82142	0.82106	0.14726	0.15551	-28.25327	-30.02644
5.70000	0.81504	0.81451	0.12706	0.13422	-24.23501	-25.75075
5.80000	0.81781	0.81713	0.11370	0.11970	-21.40722	-22.65000
5.90000	0.82877	0.82804	0.10539	0.11027	-19.44960	-20.43567
6.00000	0.84636	0.84573	0.09990	0.10382	-17.96046	-18.72861
6.10000	0.86885	0.86844	0.09518	0.09836	-16.59119	-17.18977
6.20000	0.89469	0.89459	0.08983	0.09249	-15.13142	-15.60603
6.30000	0.92267	0.92289	0.08328	0.08555	-13.52701	-13.91188
6.40000	0.95184	0.95230	0.07565	0.07762	-11.84303	-12.15757
6.50000	0.98138	0.98196	0.06756	0.06920	-10.19920	-10.44945

TABLE 12 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

T=143.00 ^{0}K RHO=0.9100 GM/CC

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K	U(R)/K CORRELATED
6.60000	1.01039	1.01093	0.05968	0.06093	-8.70597	-8.88934
6.70000	1.03773	1.03812	0.05248	0.05327	-7.42091	-7.53217
6.80000	1.06206	1.06220	0.04601	0.04627	-6.33317	-6.36956
6.90000	1.08191	1.08181	0.03990	0.03964	-5.37358	-5.33796
7.00000	1.09600	1.09570	0.03352	0.03278	-4.44173	-4.34325
7.10000	1.10345	1.10305	0.02622	0.02511	-3.43948	-3.29237
7.20000	1.10407	1.10370	0.01763	0.01627	-2.30223	-2.12318
7.30000	1.09846	1.09822	0.00782	0.00633	-1.02117	-0.82625
7.40000	1.08798	1.08794	-0.00265	-0.00416	0.34772	0.54595
7.50000	1.07451	1.07467	-0.01278	-0.01426	1.69068	1.88522
7.60000	1.06010	1.06042	-0.02141	-0.02286	2.85955	3.04965
7.70000	1.04665	1.04704	-0.02750	-0.02894	3.70808	3.89825
7.80000	1.03552	1.03588	-0.03036	-0.03185	4.13262	4.33011
7.90000	1.02733	1.02758	-0.02992	-0.03149	4.10483	4.31641
8.00000	1.02195	1.02205	-0.02668	-0.02836	3.68492	3.91395
8.10000	1.01859	1.01852	-0.02167	-0.02345	3.01015	3.25497
8.20000	1.01609	1.01589	-0.01620	-0.01804	2.26233	2.51643
8.30000	1.01321	1.01295	-0.01158	-0.01340	1.62523	1.87890
8.40000	1.00900	1.00876	-0.00882	-0.01054	1.24411	1.48695
8.50000	1.00299	1.00284	-0.00843	-0.01001	1.19687	1.42032

TABLE 12 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

T=133.00 ^{0}K RHO=1.0540 GM/CC

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K	U(R)/K CORRELATED
0.0	-0.83633	-0.96151	-10.69284	-11.07062		
0.10000	-0.78109	-0.90413	-10.59718	-10.97380		
0.20000	-0.62406	-0.74058	-10.32089	-10.69376		
0.30000	-0.38976	-0.49514	-9.89429	-10.26018		
0.40000	-0.11429	-0.20374	-9.36257	-9.71743		
0.50000	0.16080	0.09199	-8.77872	-9.11777		
0.60000	0.39557	0.35155	-8.19544	-8.51369		
0.70000	0.55831	0.54198	-7.65748	-7.95037		
0.80000	0.63051	0.64285	-7.19557	-7.45985		
0.90000	0.60943	0.64895	-6.82307	-7.05755		
1.00000	0.50777	0.57023	-6.53571	-6.74178		
1.10000	0.35062	0.42916	-6.31443	-6.49617		
1.20000	0.17036	0.25606	-6.13047	-6.29436		
1.30000	0.00043	0.08325	-5.95200	-6.10608		
1.40000	-0.13079	-0.06079	-5.75064	-5.90342		
1.50000	-0.20489	-0.15626	-5.50698	-5.66618		
1.60000	-0.21627	-0.19494	-5.21391	-5.38524		
1.70000	-0.17233	-0.18084	-4.87740	-5.06360		
1.80000	-0.09129	-0.12838	-4.51448	-4.71489		
1.90000	0.00214	-0.05869	-4.14922	-4.35982		
2.00000	0.08215	0.00526	-3.80724	-4.02128		
2.10000	0.12730	0.04374	-3.51020	-3.71921		

TABLE 12 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

T=133.00 ^{0}K RHO=1.0540 GM/CC

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K	U(R)/K CORRELATED
2.20000	0.12510	0.04454	-3.27103	-3.46618		
2.30000	0.07463	0.00570	-3.09105	-3.26444		
2.40000	-0.01293	-0.06384	-2.95941	-3.10523		
2.50000	-0.11634	-0.14582	-2.85488	-2.97017		
2.60000	-0.20805	-0.21590	-2.74970	-2.83463		
2.70000	-0.25928	-0.24829	-2.61467	-2.67225		
2.80000	-0.24533	-0.22049	-2.42452	-2.45997		
2.90000	-0.15013	-0.11766	-2.16267	-2.18239		
3.00000	0.03072	0.06447	-1.82432	-1.83482		
3.10000	0.28886	0.31847	-1.41761	-1.42451		
3.20000	0.60436	0.62608	-0.96251	-0.96978	126.70416	124.44660
3.30000	0.94870	0.96082	-0.48776	-0.49737	55.17381	55.48258
3.40000	1.28910	1.29194	-0.02644	-0.03838	2.69999	3.89336
3.50000	1.59335	1.58892	0.38896	0.37629	-37.22144	-35.94529
3.60000	1.83446	1.82580	0.73120	0.72041	-67.62796	-66.74158
3.70000	1.99405	1.98453	0.98195	0.97586	-90.19244	-90.00768
3.80000	2.06444	2.05703	1.13375	1.13476	-105.95983	-106.69065
3.90000	2.04879	2.04557	1.19026	1.19983	-115.68077	-117.46843
4.00000	1.95973	1.96156	1.16475	1.18313	-119.99795	-122.92064
4.10000	1.81660	1.82316	1.07731	1.10359	-119.57154	-123.64680
4.20000	1.64203	1.65201	0.95134	0.98368	-115.17680	-120.36024
4.30000	1.45846	1.46997	0.80990	0.84598	-107.78056	-113.96346

TABLE 12 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

T=133.00 °K RHO=1.0540 GM/CC

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K	U(R)/K CORRELATED
4.40000	1.28509	1.29611	0.67268	0.71016	-98.57711	-105.58824
4.50000	1.13578	1.14460	0.55383	0.59079	-88.93526	-96.55667
4.60000	1.01813	1.02367	0.46105	0.49628	-80.20096	-88.20736
4.70000	0.93368	0.93559	0.39586	0.42896	-73.36548	-81.58155
4.80000	0.87903	0.87770	0.35481	0.38611	-68.74895	-77.09371
4.90000	0.84762	0.84397	0.33129	0.36163	-65.92526	-74.40805
5.00000	0.83165	0.82687	0.31755	0.34797	-63.97208	-72.63907
5.10000	0.82381	0.81909	0.30650	0.33792	-61.88547	-70.75320
5.20000	0.81861	0.81484	0.29299	0.32592	-58.92362	-67.93596
5.30000	0.81295	0.81065	0.27439	0.30882	-54.76609	-63.78498
5.40000	0.80620	0.80538	0.25058	0.28595	-49.50891	-58.33044
5.50000	0.79959	0.79994	0.22332	0.25864	-43.56069	-51.94482
5.60000	0.79548	0.79641	0.19540	0.22945	-37.49056	-45.19736
5.70000	0.79635	0.79726	0.16964	0.20123	-31.86126	-38.68909
5.80000	0.80409	0.80447	0.14813	0.17630	-27.08041	-32.89959
5.90000	0.81946	0.81906	0.13173	0.15590	-23.30857	-28.08176
6.00000	0.84196	0.84080	0.12001	0.14006	-20.45254	-24.23454
6.10000	0.87000	0.86836	0.11149	0.12770	-18.23885	-21.15622
6.20000	0.90135	0.89963	0.10414	0.11710	-16.32908	-18.54759
6.30000	0.93359	0.93223	0.09598	0.10641	-14.42870	-16.11938
6.40000	0.96463	0.96397	0.08559	0.09415	-12.35748	-13.66953
6.50000	0.99302	0.99321	0.07243	0.07965	-10.07320	-11.11754

TABLE 12 (CONTINUED)

COMPARISON OF ARGON PROPERTIES

T=133.00 ^{0}K RHO=1.0540 GM/CC

R ANGSTROMS	G(R)	G(R) CORRELATED	C(R)	C(R) CORRELATED	U(R)/K	U(R)/K CORRELATED
6.60000	1.01807	1.01905	0.05695	0.06309	-7.65673	-8.50054
6.70000	1.03978	1.04127	0.04041	0.04551	-5.27245	-5.94313
6.80000	1.05856	1.06020	0.02452	0.02842	-3.11727	-3.61324
6.90000	1.07497	1.07636	0.01101	0.01347	-1.36980	-1.67511
7.00000	1.08937	1.09020	0.00122	0.00203	-0.14926	-0.24818
7.10000	1.10175	1.10185	-0.00423	-0.00515	0.50911	0.62057
7.20000	1.11165	1.11106	-0.00552	-0.00811	0.65857	0.96670
7.30000	1.11827	1.11719	-0.00360	-0.00759	0.42690	0.90035
7.40000	1.12068	1.11942	0.00009	-0.00493	-0.01083	0.58397
7.50000	1.11807	1.11698	0.00391	-0.00170	-0.46558	0.20199
7.60000	1.11002	1.10938	0.00638	0.00059	-0.76688	-0.07110
7.70000	1.09667	1.09664	0.00649	0.00081	-0.78964	-0.09872
7.80000	1.07877	1.07935	0.00382	-0.00160	-0.47172	0.19762
7.90000	1.05761	1.05865	-0.00143	-0.00661	0.17945	0.82822
8.00000	1.03483	1.03607	-0.00853	-0.01362	1.09242	1.73683
8.10000	1.01217	1.01331	-0.01649	-0.02167	2.14896	2.81425
8.20000	0.99122	0.99200	-0.02422	-0.02969	3.21046	3.92217
8.30000	0.97319	0.97344	-0.03083	-0.03671	4.14799	4.92276
8.40000	0.95881	0.95851	-0.03575	-0.04202	4.86834	5.70702
8.50000	0.94829	0.94754	-0.03877	-0.04532	5.32895	6.21415

Appendix E

Computer Programs

TABLE E 1

MOLECULAR SCATTERING FACTORS PROGRAM LISTING

```
C   MOLECULAR SCATTERING FACTORS USING GAUSSIAN BASIS FUNCTIONS TRANSFCRMED
C   FROM SLATER TYPE ORBITALS
C   7 MARCH 1971          M. PILIAVIN DEPT ENG SCI CIT
C   READ IN VALUES OF INTERNUCLEAR SEPARATION RC IN ATCMIC UNITS                C
C
C   READ IN COEFFICIENTS OF GAUSSIAN EXPANSICN IN ORDER OF INCREASING ORBITAL  C
C   ENERGY I.E. COEFF FOR 1S THEN 2S ETC.                                       C
C
C   READ IN EXPCNENTS  IN THE SAME ORDER                                        C
C
C
C   PROGRAM ASSUMES SLATER  1S ORBITALS ARE EXPANDED WITH 10 1S GAUSSIANS       C
C   PROGRAM ASSUMES SLATER  2S ORBITALS ARE EXPANDED WITH  4 1S GAUSSIANS       C
C   PROGRAM ASSUMES SLATER  2P ORBITALS ARE EXPANDED WITH  6 2P GAUSSIANS       C
C   PROGRAM ASSUMES SLATER  3S ORBITALS ARE EXPANDED WITH  4 1S GAUSSIANS       C
C   PROGRAM ASSUMES SLATER  3P ORBITALS ARE EXPANDED WITH  4 2P GAUSSIANS       C
C
C
C
C   IF MOL ORBS ARE PI TYPE THEN ISPI=1; CTHERWISE =0
C
C
C
      COMMON/BLOCK1/NBETA,NDRO,NR,NK,NPSI,NPRNT
      COMMCN/BLOCK2/RD(20),BETA(120),B(120),X(250),XA(250)
      COMMON/BLOCK3/T(100,100),EN(100,100),SPRUP(250),SPROP2(250),FATOM(
     #250)
      COMMCN/BLCCK4/AYRE(100,100),NL(20),NU(20),CAPRE(35,35)
      COMMON/BLOCK5/C(18),NTOT
      CCMMCN/BLCCK6/ XL,XR,YT,YD
      COMMCN/BLCK10/DELFRE(250),DELFIM(250),OVALAP
      COMMCN/BLOK11/TITLE(20)
      COMMCN/BLOCKA/AATAN(250),FATCM2(250),FACTEF(250),PERER(250)
```

MOLECULAR SCATTERING FACTORS PROGRAM LISTING

```
      COMMCN/ATRAN/A
      COMMCN/HANG1/ANG,ISPI
      DIMENSION D(2),SLATE(9),BETS(120),TITTY(20)
C
C
C
C
C
      EXTERNAL DUMP
      CALL ERRSET(209,2,0,0,DUMP)
C
C   REAC IN NUMBER OF EACH TYPE OF SLATER AO ON EACH CENTER
C
C
      REAC(5,1000) N1S,N2S,N3S,N2P,N3P,N3D
 1000 FORMAT(6I5)
C
C
C
      READ(5,1) NDRC,NR,NK,NPSI,NPRNT,PSII
 1    FORMAT(5I4,E15.8)
C
C
C
      REAC(5,2) H
 2    FCRMAT(E15.8)
C
      READ(5,175) (RD(M),M=1,NR)
 175  FORMAT(8F10.4)
C
C
      NSLCT=N1S+N2S+N3S+N2P+N3D+N3P
      NTOT=2*NSLOT
```

TABLE E 1 (continued)

MOLECULAR SCATTERING FACTORS PROGRAM LISTING

```
C
      READ(5,10) (NL(I),I=1,NTOT),(NU(J),J=1,NTOT)
   10 FORMAT(20I4)
C
C
C    READ IN COEFF OF GAUSSIAN EXPANSION OF THE SLATER ORBITALS
C    A COMPLETE SET IS REQUIRED FOR EACH TYPE OF SLATER ORBITAL I.E. IF
C    TWO SLATER ORBITALS ON THE CENTER TWO COMPLETE SETS OF COEFFICIENTS ARE
C    REQUIRED.
C
      NTOTG=N1S*10+N2S*4+N3S*4+N2P*6+N3P*4+N3D*0
C
      READ(5,200) (B(I),I=1,NTOTG)
 200  FORMAT (5E15.8)
      DO 2050 IJ=1,NTOTG
 2050 B(IJ+NTOTG)=B(IJ)
C
C
      NBETA=2*NTOTG
C
C
C    READ IN EXPONENTS
C
C
      READ(5,150) (BETS(J),J=1,NTOTG)
 150  FORMAT(5E15.8)
C
C
C
C
C
C
C
```

MOLECULAR SCATTERING FACTORS PROGRAM LISTING

```
C
      DO 25 I=1,NR
      R=RD(I)
      READ(5,261) TITLE
 261  FORMAT(20A4)
C
C
C
C    READ IN EXPONENTS OF SLATER ORBITALS
C
      READ(5,220) SLATE
 220  FORMAT(8F10.5)
C
      WRITE(6,2900)
 2900 FORMAT(1H1//20X,'COEFFICIENTS OF SLATER ATOMIC ORBS ON EACH CENTER
     #',//11X,'LEFT',22X,'RIGHT',//)
C
      DO 1010 JX=1,NSLOT
C
      READ(5,15) C(JX),NG,NUG,ISPI
 15   FORMAT(E15.8,3I5)
C
      JT=JX+NSLOT
      C(JX+NSLOT)=C(JX)*NG-C(JX)*NUG
      WRITE(6,2901) JX,C(JX),JT,C(JT)
 2901 FORMAT(5X,'C(',I2,')=',E15.8,5X,'C(',I2,')=',E15.8)
 1010 CONTINUE
C
      PSI=PSII+1.570796*ISPI
      ANG=COS(PSI)
C
C THERE ARE THREE TITLE CARDS GIVING INFORMATION REGARDING PSI,,R,ETC
C    WHICH ATE READ INTO DUMMY TITLE STORAGE TITTY
```

TABLE E 1 (continued)

MCLECULAR SCATTERING FACTCRS PROGRAM LISTING

```
      READ(5,261) TITTY
      READ(5,261) TITTY
      READ(5,261) TITTY
C
      READ(5,1100) (FATOM(JJ),JJ=1,NK)
 1100 FORMAT(8F10.7)
C
C
C
C
C   RECOMPUTING EXPCNENTS FOR GAUSSIAM EXPANSION OF      1S 1
C
      DO 300 JC=1,10
      BETA(JC)=BETS(JC)*(SLATE(1)*SLATE(1))
 300  BETA(JC+NTOTG)=BETA(JC)
C
C
C
C   RECOMPUTING EXPONENTS FOR GAUSSIAM EXPANSION OF      2S 1
C
      DO 301 JC=11,14
      BETA(JC)=BETS(JC)*(SLATE(2)*SLATE(2))*4.
 301  BETA(JC+NTOTG)=BETA(JC)
C
C
C
C
C   RECOMPUTING EXPCNENTS FOR GAUSSIAM EXPAKSION OF      2S 2
C
      DO 302    JC=15,18
      BETA(JC)=BETS(JC)*(SLATE(3)*SLATE(3))*4.
 302  BETA(JC+NTOTG)=BETA(JC)
C
```

MOLECULAR SCATTERING FACTORS PROGRAM LISTING

```
C
C   RECOMPUTING EXPONENTS FOR GAUSSIAM EXPANSION OF      2P 1
C
C
      DO 303 JC=19,24
      BETA(JC)=BETS(JC)*(SLATE(4)*SLATE(4))*4.
 303  BETA(JC+NTOTG)=BETA(JC)
C
C
C   RECOMPUTING EXPONENTS FOR GAUSSIAM EXPAKSION OF      2P 2
C
C
      DO 304 JC=25,30
      BETA(JC)=BETS(JC)*(SLATE(5)*SLATE(5))*4.
 304  BETA(JC+NTOTG)=BETA(JC)
C
C
C   RECOMPUTING EXPONENTS FOR GAUSSIAM EXPANSION OF      3S 1
C
C
      DO 305 JC=31,34
      BETA(JC)=BETS(JC)*(SLATE(6)*SLATE(6))*9.
 305  BETA(JC+NTOTG)=BETA(JC)
C
C
C   RECCMPUTING EXPONENTS FOR GAUSSIAM EXPANSION OF      3S 2
C
C
      DO 306 JC=35,38
      BETA(JC)=BETS(JC)*(SLATE(7)*SLATE(7))*9.
 306  BETA(JC+NTOTG)=BETA(JC)
C
C
```

TABLE E 1 (continued)

MOLECULAR SCATTERING FACTORS PROGRAM LISTING

```
C   RECCMPUTING EXPONENTS FOR GAJSSIAM EXPANSION OF     3P 1
C
C
      DO 307 JC=39,42
      BETA(JC)=BETS(JC)*(SLATE(8)*SLATE(8))*9.
 307  BETA(JC+NTOTG)=BETA(JC)
C
C
C   RECOMPUTING EXPONENTS FOR GAUSSIAM EXPANSION OF     3P 2
C
C
      DO 308 JC=43,46
      BETA(JC)=BETS(JC)*(SLATE(9)*SLATE(9))*9.
 308  BETA(JC+NTOTG)=BETA(JC)
C
C
C
C
C
C
C
      DO 3 M=1,NBETA
      DO 4 J=1,NBETA
      T(J,M)=BETA(M)+BETA(J)
      EN(J,M)=((4.*BETA(M)*BETA(J))/(T(J,M)*T(J,M)))**.75
    4 CONTINUE
    3 CONTINUE
C
C
C
C
      DO 30 K=1,NK
      X(K)=.0052917*(K-1)*H
```

MOLECULAR SCATTERING FACTORS PRCGRAM LISTING

```
      XA(K)=X(K)/(.529170)
      EX=X(K)
      A=2.0*3.14159265*EX*R*ANG
C
C
C
           CALL S1AS1A(A,R,AYRE, 1,18, 1,18)
C
           CALL S1AP2A(A,R,AYRE, 1,18,19,30)
C
           CALL S1AS1A(A,R,AYRE, 1,18,31,38)
C
           CALL S1AP2A(A,R,AYRE, 1,18,39,46)
C
           CALL S1AS1B(A,R,AYRE, 1,18,47,64)
C
           CALL S1AP2B(A,R,AYRE, 1,18,65,76)
C
           CALL S1AS1B(A,R,AYRE, 1,18,77,84)
C
           CALL S1AP2B(A,R,AYRE, 1,18,85,92)
C
           CALL P2AP2A(A,R,AYRE,19,30,19,30)
C
           CALL S1AP2A(A,R,AYRE,19,30,31,38)
C
           CALL P2AP2A(A,R,AYRE,19,30,39,46)
C
           CALL P2AS1B(A,R,AYRE,19,30,47,64)
C
           CALL P2AP2B(A,R,AYRE,19,30,65,76)
C
           CALL P2AS1B(A,R,AYRE,19,30,77,84)
```

TABLE E 1 (continued)

MOLECULAR SCATTERING FACTORS PROGRAM LISTING

```
C
           CALL P2AP2B(A,R,AYRE,19,30,85,92)
C
           CALL S1AS1B(A,R,AYRE,31,38,47,64)
C
           CALL S1AS1A(A,R,AYRE,31,38,31,38)
C
           CALL S1AP2A(A,R,AYRE,31,38,39,46)
C
           CALL S1AP2B(A,R,AYRE,31,38,65,76)
C
           CALL S1AS1B(A,R,AYRE,31,38,77,84)
C
           CALL S1AP2B(A,R,AYRE,31,38,85,92)
C
           CALL P2AP2A(A,R,AYRE,39,46,39,46)
C
           CALL P2AS1B(A,R,AYRE,39,46,47,64)
C
           CALL P2AP2B(A,R,AYRE,39,46,65,76)
C
           CALL P2AS1B(A,R,AYRE,39,46,77,84)
C
           CALL P2AP2B(A,R,AYRE,39,46,85,92)
C
           CALL S1BS1B(A,R,AYRE,47,64,47,64)
C
           CALL S1BP2B(A,R,AYRE,47,64,65,76)
C
           CALL S1BS1B(A,R,AYRE,47,64,77,84)
C
           CALL S1BP2B(A,R,AYRE,47,64,85,92)
C
```

MOLECULAR SCATTERING FACTORS PROGRAM LISTING

```
           CALL P2BP2B(A,R,AYRE,65,76,65,76)
C
           CALL S1BP2B(A,R,AYRE,65,76,77,84)
C
           CALL P2BP2B(A,R,AYRE,65,76,85,92)
C
           CALL S1BS1B(A,R,AYRE,77,84,77,84)
C
           CALL S1BP2B(A,R,AYRE,77,84,85,92)
C
           CALL P2BP2B(A,R,AYRE,85,92,85,92)
C
C
C
      CALL BBSUM
C
C
C
      IF(K.GT.NPRNT) GO TO 50
C
C
      WRITE(6,100)
  100 FORMAT(/40X,'   INDIVIDUAL BASIS INTEGRALS, CAPRE(I,J) ')
C
C
      WRITE(6,101) RD(I),X(K)
  101 FORMAT(//30X,'    R=',E15.8,5X,'X=',E15.8,/)
C
      DO 120 L=1,NTOT
C
      WRITE(6,115) L
  115 FORMAT(/20X,I4,/)
C
```

TABLE E 1 (continued)

MOLECULAR SCATTERING FACTCRS PRCGRAM LISTING

```
C
      WRITE(6,110) (CAPRE(L,J),J=1,NTOT)
 110  FORMAT(3X,9(E11.4,3X),/6X,9(E11.4,3X),/)
C
C
C
 120  CCNTINUE
C
C
 50   CONTINUE
      Ih=I
      IF(K.EQ.1) ANORM=BASINT(RD(I),1,ANG,H,IW)
       SPROP(K)=BASINT(RD(I),K,ANG,H,IW)/ANORM
      FAT=FATOM(K)*COS(A)
      DELFRE(K)=(SPROP(K)-FAT)*COS(A)
      DELFIM(K)=(SPROP(K)-FAT)*COS(A)
      WRITE(6,2002)  XA(K), FAT
 2002 FORMAT(/30X,'SIN(THETA)/LAMBCA =',E15.8,'    F MOL CENT=',E15.8)
 30   CCNTINUE
C
C
C
C
C
      WRITE(6,136)
 136  FORMAT(1H1//35X,' MOLECULAR SCATTERING FACTORS ' )
C
C
      WRITE(6,171) TITLE
 171  FORMAT(//10X,20A4)
C
      WRITE(6,172) ANCRM
 172  FORMAT(//37X,'NORMALIZATION CONSTANT = ',E15.8)
```

MOLECULAR SCATTERING FACTCRS PRCGRAM LISTING

```
C
      WRITE(6,118) PSII,RD(I)
 118  FORMAT(//35X,'PSI= ',E15.8,30X,'R= ',E15.8)
C
C
      WRITE(6,116)
 116  FORMAT(/17X,'SIN(THETA)/LAMBCA',9X,'FACTOR',17X,'SIN(THETA)/LAMBDA
     @',9X,'FACTOR')
C
C
      WRITE(6,156) (XA(JK),SPROP(JK), JK=1,NK )
 156  FORMAT(5X,4E25.8)
C
C
      IF(NPSI.EQ.0) GO TO 656
      CALL PONCHO(I,PSII,NK)
 656  CONTINUE
  25  CONTINUE
      STOP
      END
      FUNCTION BASINT(ERD,K,ANG,H,NI)
      COMMON/BLOCK1/NBETA,NDRU,NR ,NK,NPSI ,NPRNT
      CCMMON/BLOCK3/T(100,100),EN(100,100),SPROP(250),SPROP2(250),FATOM(
     #250)
      COMMCN/BLOCK4/AYRE(100,100),NL(20),NU(20),CAPRE(35,35)
      CCMMCN/BLOCK5/C(18),NTOT
      COMMCN/BLOK10/DELFRE(250),DELFIM(250),OVALAP
      COMMON/BLOCKA/AATAN(250),FATOM2(250),FACTEF(250),PERER(250)
C
      R=ERD
C
      AB=2.*3.14159265*R*ANG*(.0052917)*(K-1)*H
C
```

TABLE E 1 (continued)

MOLECULAR SCATTERING FACTORS PROGRAM LISTING

```
      SUMRE=0.0
      DO 1 I=1,NTOT
      DO 2 J=1,NTOT
      SUMRE=SUMRE+C(I)*C(J)*CAPRE(I,J)
    2 CONTINUE
    1 CONTINUE
C
C
C
      BASINT=SUMRE
C
      CONTINUE
      RETURN
      END
      SUBROUTINE S1AS1A(A,R,AYRE,NL1,NU1,NL2,NU2)
C
C
      COMMON/BLOCK2/RD(20),BETA(120),B(120),X(250),XA(250)
      COMMON/BLOCK3/T(100,100),EN(100,100),SPROP(250),SPROP2(250),FATOM(
     #250)
      COMMON/HANG1/ANG
      DIMENSION AYRE(100,100)
C
C
C   THIS SUBROUTINE COMPUTES THE MATRIX ELEMENTS OF THE SCATTERING OPERATOR     C
C   FOR GAUSSIAN ORBITALS OF TYPE  1S,CENTER A AND TYPE 1S,CENTER A
C
C
      DO 4 J=NL1,NU1
      DO 5 M=NL2,NU2
      P=-((A/(R*ANG))**2)/(T(J,M))
      AYRE(J,M)=EN(J,M)*EXP(P)*COS(A)
      AYRE(M,J)=AYRE(J,M)
```

MOLECULAR SCATTERING FACTORS PROGRAM LISTING

```
C
    5 CONTINUE
    4 CONTINUE
C
      RETURN
      END
      SUBROUTINE S1AP2A(A,R,AYRE,NL1,NU1,NL2,NU2)
C
C
      COMMON/BLOCK2/RD(20),BETA(120),B(120),X(250),XA(250)
      COMMON/BLOCK3/T(100,100),EN(100,100),SPROP(250),SPROP2(250),FATOM(
     #250)
      COMMON/HANG1/ANG
      DIMENSION AYRE(100,1)
C
C
C   THIS SUBROUTINE COMPUTES THE MATRIX ELEMENTS OF THE SCATTERING OPERATOR     C
C   FOR GAUSSIAN ORBITALS OF TYPE  1S,CENTER A AND TYPE 2P,CENTER A
C
C
      DO 4 J=NL1,NU1
      DO 5 M=NL2,NU2
      P=-((A/(R*ANG))**2)/(T(J,M))
      AYRE(J,M)=EN(J,M)*2.0*SQRT(BETA(M))*EXP(P)*A*(SIN(A))/(R*T(J,M))
      AYRE(M,J)=AYRE(J,M)
    5 CONTINUE
    4 CONTINUE
C
      RETURN
      END
      SUBROUTINE S1AS1B(A,R,AYRE,NL1,NU1,NL2,NU2)
C
C
```

TABLE E 1 (continued)

MOLECULAR SCATTERING FACTCRS PROGRAM LISTING

```
      CCMMCN/BLOCK2/RC(20),BETA(120),B(120),X(250),XA(250)
      COMMON/BLOCK3/T(100,100),EN(100,100),SPROP(250),SPROP2(250),FATOM(
     #250)
      COMMCN/HANG1/ANG
      DIMENSION AYRE(100,1)
C
C
C   THIS SUBROUTINE COMPUTES THE MATRIX ELEMENTS OF THE SCATTERING OPERATOR     C
C   FOR GAUSSIAN ORBITALS OF TYPE  1S,CENTER A AND TYPE 1S,CENTER B             C
C
C
      DO 4 J=NL1,NU1
      DO 5 M=NL2,NU2
      P=-((A/(R*ANG))**2)/(T(J,M))
      P2=-BETA(M)*BETA(J)*R*R/T(J,M)
      AYRE(J,M)=EN(J,M)*EXP(P2)*EXP(P)*
     1COS(A*(BETA(M)-BETA(J))/T(J,M))
      AYRE(M,J)=AYRE(J,M)
    5 CCNTINUE
    4 CONTINUE
C
      RETURN
      END
      SUBROUTINE S1AP2B(A,R,AYRE,NL1,NU1,NL2,NU2)
C
C
      COMMON/BLOCK2/RD(20),BETA(120),B(120),X(250),XA(250)
      CCMMCN/BLOCK3/T(100,100),EN(100,100),SPROP(250),SPROP2(250),FATOM(
     #250)
      COMMCN/HANG1/ANG
      DIMENSION AYRE(100,1)
C
C
```

MOLECULAR SCATTERING FACTCRS PRCGRAM LISTING

```
C   THIS SUBROUTINE CCMPUTES THE MATRIX ELEMENTS OF THE SCATTERING OPERATOR     C
C   FOR GAUSSIAN ORBITALS OF TYPE  1S,CENTER A AND TYPE 2P,CENTER B
C
C
      DO 4 J=NL1,NU1
      DO 5 M=NL2,NU2
      P=-((A/(R*ANG))**2)/(T(J,M))
      P2=-BETA(M)*BETA(J)*R*R/T(J,M)
      CKOS=COS(A*(BETA(M)-BETA(J))/T(J,M))
      SINE=SIN(A*(BETA(M)-BETA(J))/T(J,M))
      COFRE=(-1)*((BETA(J)*R/T(J,M))*CKOS+(A/(R*T(J,M)))*SINE)
      SUP=EN(J,M)*2.0*SQRT(BETA(M))*EXP(P)*EXP(P2)
      AYRE(J,M)=SUP*COFRE
      AYRE(M,J)=AYRE(J,M)
    5 CONTINUE
    4 CONTINUE
C
      RETURN
      END
      SUBROUTINE P2AP2A(A,R,AYRE,NL1,NU1,NL2,NU2)
C
C
      COMMCN/BLOCK2/RD(20),BETA(120),B(120),X(250),XA(250)
      CCMMCN/BLCCK3/T(100,100),EN(100,100),SPROP(250),SPROP2(250),FATOM(
     #250)
      COMMCN/HANG1/ANG
      DIMENSION AYRE(100,1)
C
C
C   THIS SUBROUTINE COMPUTES THE MATRIX ELEMENTS OF THE SCATTERING OPERATOR     C
C   FOR GAUSSIAN ORBITALS OF TYPE  2P,CENTER A AND TYPE 2P,CENTER A
C
C
```

TABLE E 1 (continued)

MOLECULAR SCATTERING FACTORS PROGRAM LISTING

```
      DO 4 J=NL1,NU1
      DO 5 M=NL2,NU2
      P=-((A/(R*ANG))**2)/(T(J,M))
      COF=1/(2.0*T(J,M))-A*A/(R*R*T(J,M)*T(J,M))
      AYRE(J,M)=EN(J,M)*4.0*SQRT(BETA(J)*BETA(M))*EXP(P)*COS(A)*COF
      AYRE(M,J)=AYRE(J,M)
      AYRE(M,J)=AYRE(J,M)
    5 CONTINUE
    4 CCNTINUE
C
      RETURN
      END
      SUBROUTINE P2AS1B(A,R,AYRE,NL1,NU1,NL2,NU2)
C
C
      COMMCN/BLOCK2/RD(20),BETA(120),B(120),X(250),XA(250)
      COMMCN/BLOCK3/T(100,100),EN(100,100),SPROP(250),SPROP2(250),FATOM(
     #250)
      COMMCN/HANG1/ANG
      DIMENSION AYRE(100,1)
C
C
C    THIS SUBROUTINE CCMPUTES THE MATRIX ELEMENTS OF THE SCATTERING OPERATOR    C
C    FOR GAUSSIAN ORBITALS OF TYPE  2P,CENTER A AND TYPE 1S,CENTER B
C
C
      DO 4 J=NL1,NU1
      DO 5 M=NL2,NU2
      P=-((A/(R*ANG))**2)/(T(J,M))
      P2=-BETA(M)*BETA(J)*R*R/T(J,M)
      CKCS=COS(A*(BETA(M)-BETA(J))/T(J,M))
      SINE=SIN(A*(BETA(M)-BETA(J))/T(J,M))
      COERE=(BETA(M)*R/T(J,M))*CKOS-(A/(R*T(J,M)))*SINE
```

MOLECULAR SCATTERING FACTCRS PRCGRAM LISTING

```
      SUP=EN(J,M)*2.0*SQRT(BETA(J))*EXP(P)*EXP(P2)
      AYRE(J,M)=SUP*COERE
      AYRE(M,J)=AYRE(J,M)
    5 CONTINUE
    4 CONTINUE
C
      RETURN
      END
      SUBROUTINE P2AP2B(A,R,AYRE,NL1,NU1,NL2,NU2)
C
C
      COMMCN/BLOCK2/RD(20),BETA(120),B(120),X(250),XA(250)
      COMMCN/BLCCK3/T(100,100),EN(100,100),SPROP(250),SPROP2(250),FATOM(
     #250)
      CCMMCN/HANG1/ANG,ISPI
      DIMENSICN AYRE(100,1)
C
C
C    THIS SUBROUTINE CCMPUTES THE MATRIX ELEMENTS OF THE SCATTERING OPERATOR    C
C    FOR GAUSSIAN ORBITALS OF TYPE  2P,CENTER A AND TYPE 2P,CENTER B
C
C
      DO 4 J=NL1,NU1
      DO 5 M=NL2,NU2
      P=-((A/(R*ANG))**2)/(T(J,M))
      P2=-BETA(M)*BETA(J)*R*R/T(J,M)
      CKOS=COS(A*(BETA(M)-BETA(J))/T(J,M))
      SINE=SIN(A*(BETA(M)-BETA(J))/T(J,M))
      COER=(1/(2.*T(J,M)))*(1.-(2./T(J,M))*(R*R*BETA(M)*BETA(J)+A*A/(R*R
     1)))
      COEI=(1/(T(J,M)**2))*A*(BETA(M)-BETA(J))
      COF=1/(2.0*T(J,M))-A*A/(R*R*T(J,M)*T(J,M))
      SUP=EN(J,M)*EXP(P)*EXP(P2)*4.0*SQRT(BETA(J)*BETA(M))
```

TABLE E 1 (continued)

MOLECULAR SCATTERING FACTORS PROGRAM LISTING

```
      AYRE(J,M)=SUP*(COER*CKOS-COEI*SINE)*FLOAT(1-ISPI)+SUP*CKOS*COF*FLO
     #AT(ISPI)
      AYRE(M,J)=AYRE(J,M)
 5    CONTINUE
 4    CONTINUE
C
      RETURN
C
      END
      SUBROUTINE S1BS1B(A,R,AYRE,NL1,NU1,NL2,NU2)
C
      COMMON/BLOCK2/RD(20),BETA(120),B(120),X(250),XA(250)
      COMMON/BLOCK3/T(100,100),EN(100,100),SPROP(250),SPROP2(250),FATOM(
     #250)
      COMMON/HANG1/ANG
C
      DIMENSION AYRE(100,1)
C    THIS SUBROUTINE COMPUTES THE MATRIX ELEMENTS OF THE SCATTERING OPERATOR     C
C    FOR GAUSSIAN ORBITALS OF TYPE  1S,CENTER B AND TYPE 1S,CENTER B
C
C
      DO 4 J=NL1,NU1
      DO 5 M=NL2,NU2
      P=-((A/(R*ANG))**2)/(T(J,M))
      AYRE(J,M)=EN(J,M)*EXP(P)*COS(A)
      AYRE(M,J)=AYRE(J,M)
 5    CONTINUE
 4    CONTINUE
C
      RETURN
      END
      SUBROUTINE S1BP2B(A,R,AYRE,NL1,NU1,NL2,NU2)
C
```

MOLECULAR SCATTERING FACTORS PROGRAM LISTING

```
C
      COMMON/BLOCK2/RD(20),BETA(120),B(120),X(250),XA(250)
      COMMON/BLOCK3/T(100,100),EN(100,100),SPROP(250),SPROP2(250),FATOM(
     #250)
      COMMON/HANG1/ANG
      DIMENSION AYRE(100,1)
C
C
C    THIS SUBROUTINE COMPUTES THE MATRIX ELEMENTS OF THE SCATTERING OPERATOR     C
C    FOR GAUSSIAN ORBITALS OF TYPE  1S,CENTER B AND TYPE 2P,CENTER B
C
C
      DO 4 J=NL1,NU1
      DO 5 M=NL2,NU2
      P=-((A/(R*ANG))**2)/(T(J,M))
      AYRE(J,M)=EN(J,M)*2.0*SQRT(BETA(M))*EXP(P)*(-1)*A*(SIN(A))/
     1(R*T(J,M))
      AYRE(M,J)=AYRE(J,M)
C
 5    CONTINUE
 4    CONTINUE
      RETURN
      END
      SUBROUTINE P2BP2B(A,R,AYRE,NL1,NU1,NL2,NU2)
C
C
      COMMON/BLOCK2/RD(20),BETA(120),B(120),X(250),XA(250)
      COMMON/BLOCK3/T(100,100),EN(100,100),SPROP(250),SPROP2(250),FATOM(
     #250)
      COMMON/HANG1/ANG
      DIMENSION AYRE(100,1)
C
C
```

TABLE E 1 . (continued)

MOLECULAR SCATTERING FACTCRS PRCGRAM LISTING

```
C   THIS SUBROUTINE COMPUTES THE MATRIX ELEMENTS OF THE SCATTERING OPERATOR    C
C   FOR GAUSSIAN ORBITALS OF TYPE  2P,CENTER B AND TYPE 2P,CENTER B
C
C
      DO 4 J=NL1,NU1
      DO 5 M=NL2,NU2
      P=-((A/(R*ANG))**2)/(T(J,M))
      COF= 1/(2.*T(J,M)) - (A*A/(R*R*T(J,M)*T(J,M)))
      AYRE(J,M)=EN(J,M)*4.*SQRT(BETA(J)*BETA(M))*EXP(P)*COS(A)*COF
      AYRE(M,J)=AYRE(J,M)
 5    CONTINUE
 4    CONTINUE
C
      RETURN
      END
      SUBRCUTINE BBSUM
      COMMCN/BLOCK1/NBETA,NDRO,NR,NK,NPSI,NPRNT
      COMMCN/BLOCK2/RD(20),BETA(120),B(120),X(250),XA(250)
      COMMCN/BLOCK3/T(100,100),EN(100,100),SPROP(250),SPROP2(250),FATOM(
     #250)
      COMMCN/BLOCK4/AYRE(100,100),NL(20),NU(20),CAPRE(35,35)
      COMMCN/BLOCK5/C(18),NTOT
C
C
      EXTERNAL CUMP
      CALL ERRSET(209,2,0,0,DUMP)
C
      DC 50 I=1,NTOT
      NA1=NL(I)
      NB1= NU(I)
      DO 55 K=1,NTOT
      NA2=NL(K)
      NB2=NU(K)
```

MOLECULAR SCATTERING FACTCRS PRCGRAM LISTING

```
      SUMRE=0.0
      DO 60 L=NA1,NB1
      DO 65 M=NA2,NB2
      SUMRE=SUMRE+B(L)*B(M)*AYRE(L,M)
   65 CONTINUE
   60 CCNTINUE
      CAPRE(I,K)=SUMRE
   55 CONTINUE
   50 CONTINUE
      RETURN
      END
      SUBRCUTINE PONCHO(II,PSI,NK)
      COMMON/BLOCK2/RD(20),BETA(120),B(120),X(250),XA(250)
      COMMON/BLOCK3/T(100,100),EN(100,100),SPROP(250),SPROP2(250),FATOM(
     #250)
      COMMCN/BLOK10/DELFRE(250),DELFIM(250),OVALAP
      CCMMCN/BLOK11/TITLE(20)
      CCMMCN/BLOCKA/AATAN(250),FATCM2(250),FACTEF(250),PERER(250)
C
C
      PUNCH 1, TITLE
 1    FORMAT(20A4)
C
C
      OVALAP=0.
      PUNCH 2,RD(II),PSI,OVALAP,NK,X(2)
 2    FORMAT('R=',F10.7,2X,'PSI=',F10.7,2X,'OVLAP=',F10.7,2X,'NUMEX=',I4
     #,2X,'DELTA-X=',F10.7)
C
C
      PUNCH 3
 3    FORMAT(5X,'MOLECULAR SCATTERING FACTOR CALCULATED AT MOLECULAR CEN
     +TER')
```

TABLE E 1 (continued)

MOLECULAR SCATTERING FACTORS PROGRAM LISTING

```
C
      PUNCH 4, (SPROP(JA),JA=1,NK)
 4    FORMAT(8F10.7)
C
      PUNCH 5
 5    FORMAT(5X,'REAL PART OF CORRECTION TO ISOLATED ATOM')
      PUNCH 4,(DELFRE(JB),JB=1,NK)
      PUNCH 6
 6    FORMAT(5X,'IMAGINARY PART OF CORRECTION TO ISOLATED ATOM')
      PUNCH 4,(DELFIM(JC),JC=1,NK)
C
      CONTINUE
      RETURN
      END
      SUBROUTINE DUMP
      CALL SNAP(1)
      STOP
      END
```

TABLE E 2

PROGRAM FOR GENERATING CORRELATION VALUES

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                              C
C                                                                              C
C                                                                              C
C   PROGRAM TO PERFORM FOURIER TRANSFORMS OF THE SCATTERING INTENSITY          C
C   WITH AND WITHOUT CORRECTED SCATTERING AFCTORS AND TO STUDY THEIR EFFECT    C
C   UPON G(R)                                                                  C
C   M. PILIAVIN, 1 OCT. 1971, DEPT. OF ENGR. AND APPLIED SCIENCE.              C
C   STRUT STORES THE READ IN STRUCTURE FACTCRS                                 C
C   SX STORES THE VALUES OF 4*PI*SIN(THETA)/LAMBDA FOR THE STRUCT FACTORS      C
C   NINV IS THE NUMBR OF ITERATICNS OF STRUCTURE FACTOR                        C
C   NSTRUT IS THE NUMBER OF POINTS IN THE STRUCTURE FACTOR CATA                C
C   NINT IS THE TOTAL NUMBER OF STRUCTURE FACTOR POINTS TO BE COMPUTED FRCM    C
C   G(R)   NXTRA IS THE EXCESS NUMBER OF STRUCTURE FACTOR POINTS TO BE         C
C   COMPUTED IN ADDITION TO NSTRUT FOR A TOTAL OF NINT                         C
C                                                                              C
C   NFR= NC. OF CONFIGURATION POINTS FOR WHICH CORRELATION AMPLITUDES R CALC   C
C   NSTRUT= NO. OF AVAILABLE STRUCTURE FACTOR POINTS                           C
C   NSL= LCWER INDEX FOR SCATTERINGE VECTOR; =1 IF S=0.                        C
C   NDELS INTERVAL FOR S INDEXES; TO OBTAIN THE PROPER VALUE OF UPPER  IMIT    C
C   S(UPPER)=4.*PI*(NSU-1)*DELX WHERE DELX IS THE SPACING OF THE CORRELATCCN   C
C   AMPLITUDE ABSCISSA.                                                        C
C   NWRIT= 0 DOES NOR WRITE OUT VALUES OF F(S) FOR THE ISLLATED ATOM           C
C   NR3= NC. OF POINTS USED TO INVERT THE STRUCTURE FACTOR.                    C
C   KEY= PUT NUMBRR OF ITERATIONS DESIRED FOR CORRELATICN STRUCTURE FACTOR.    C
C                                                                              C
C                                                                              C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C
C
      IMPLICIT REAL*8(A-H,O-Z)
C
```

PROGRAM FOR GENERATING CORRELATICN VALUES

```
C
C
      DIMENSION TITLE1(20),TITLE2(20)
      DIMENSION STRUT(151),SX(151),C(4,151),GN(151)
      DIMENSION R(151),G(151),SCAL(110),CORSTR(110),CG(4,151)
      DIMENSION TITEL1(10),TITTY(10),TIT1(15,10),TIT2(15,10)
      DIMENSION GL1(151),FREEAT(110),RR(151),YNTGND(151)
      DIMENSION RF(15),DELX(15),NFX(15),GCCOR(151)
      DIMENSION DELPAV(15,110),CORSTT(25)
      DIMENSION INT(10),YNTG2(151),CG2(4,151)
      COMMCN/A1/R,G,CG,NR
      COMMON C,DELPAV,CG2,STRUT,SX,GN,SCAL,CORSTR,GL1,FREEAT,RR,YNTGND,T
     #IT1,TIT2
C
      REAL*4 ASS(151),ORD(151)
      EXTERNAL ANY
C
      READ(5,1) NRREQ,NFR,NSTRUT,NSL,NSU,NDELS,NWRIT,NR3,KEY,NTRIP
 1    FORMAT(10I5)
C
C
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C
C
      READ(5,1100) DELRR,DELRRO
 1100 FORMAT(2F10.7)
C
      READ(5,1001) TITEL1
 1001 FORMAT(10A8)
C
```

TABLE E 2 (continued)

```
          PROGRAM FOR GENERATING CORRELATICN VALUES


C
      READ(5,1002) TEMP,RHO,DELR,NR
 1002 FORMAT(6X,F10.6,5X,F10.7,6X,F10.7,4X,I5)
C
      IF(NTRIP.EQ.0) GO TO 1200
C
      MUX=(2.D0*DELRRO/DELRR)+(2.D0*(NRREQ-1))+1.5D0
      NUX=2*MUX
      IF(NUX.LE.NR) GO TO 1200
      WRITE(6,1201) NR,NUX
 1201 FORMAT(//15X,'<<<<<< PROGRAM SELF TEST OF INPUT CATA: INSUFFICIENT
     # RADIAL DISTRIBUTION FUNCTION INPUT POINTS >>>>>>',//18X,'INPUT NU
     #MBER= ',I5,15X,'NUMBER REQUIREC = ',I5,//)
      GO TO 1350
 1200 CONTINUE
C
      READ(5,1003) (GL1(JA),JA=1,NR)
 1003 FORMAT(8F10.7)
C
C
      READ(5,2) TITLE1
 2    FCRMAT(20A4)
C
      READ(5,3) TEMP,RHO
 3    FORMAT(2F10.7)
C
      RHO=RHO*(.3010D0)/18.0D0
C
      REAC(5,4) (STRUT(JA),JA=1,NSTRUT)
 4    FORMAT(8F10.7)
C
C
      READ(5,2) TITLE2




          PROGRAM FOR GENERATING CORRELATION VALUES


C
C
C
C
      READ(5,4) (SX(JA),JA=1,NSTRUT)
C
      DO 1004 IA=1,NFR
C
C
      READ(5,1001) (TIT1(IA,JA),JA=1,10)
C
C
      READ(5,1005) RF(IA),NFX(IA),DELX(IA)
 1005 FORMAT(2X,F10.7,11X,I4,9X,F10.7)
C
C
      NFXX=NFX(IA)
C
C
      READ(5,1001) (TIT2(IA,JD),JD=1,10)
C
C
      READ(5,1003) (DELPAV(IA,JC),JC=1,NFXX)
 1004 CONTINUE
C
      READ(5,1001) TITTY
C
      READ(5,1003) (FREEAT(JA),JA=1,NFXX)
C
C
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
```

TABLE E 2 (continued)

PROGRAM FOR GENERATING CORRELATICN VALUES

```
C
C
C
      WRITE(6,101)   NSTRUT,NRREQ,DELR
 101  FORMAT(//30X,'*******  INPUT  INFORMATION  ******',//19X,' NUMBER
     #OF EXPERIMENTAL STRUCTURE FACTOR POINTS IS   ',I5,/20X,'NUMBER OF
     #RADIAL DISTRIBUTION FUNCTION POINTS TO BE GENERATED IS  ',I5,/,20X
     #,'SPACING ALONG ABSCISSA OF THE RADIAL DISTRIBUTION FUNCTION IS  '
     #,E15.8,//)
C
C
C
      DO 102 JB=1,NSTRUT
      STRUT(JB)=STRUT(JB)
      WRITE(6,201) SX(JB),STRUT(JB)
 201  FORMAT(30X,'SX=',E15.8,15X,'STRUT-1=  ',E15.8)
 102  CONTINUE
C
C
      WRITE(6,3003)
 3003 FORMAT(//)
C
      PI=3.14159265359D0
C
      YPA=0.0D0
      YPB=0.0D0
C
C
C
      DO 2010 JK=1,NFR
 2010 RF(JK)=RF(JK)*.52917D0
C
C
```

PROGRAM FOR GENERATING CORRELATICN VALUES

```
      PARAM=0.0D0
C
C
      DO 2001 JC=1,NR
C
      R(JC)=DELR*(JC-1)
C
      ASS(JC)=R(JC)
      G(JC)=GL1(JC)
C
 2001 CONTINUE
      KEYNUM=0
 8000 CONTINUE
C
      CALL SPLIN2(YPA,YPB,R,G,CG,2,2,2,NR)
C
      DO 2002 JD=NSL,NSU,NDELS
C
      SCALX=DELX(1)*(JD-1)
      SCAL(JD)=DELX(1)*(JD-1)*PI*4.0D0/.52917D0
C
C
      IF(NWRIT.NE.0) WRITE(6,2005) SCAL(JD),FREEAT(JD)
C
C
 2005 FORMAT(//25X,'INTERPOLATED VALUES OF SCATTERING CORRECTION AND G(R
     #) FOR INTEGRATION',//25X,'MAGNITUDE OF 4*PI*SIN(THETA)/LAMBCA=',E1
     #5.8,/25X,'MAGNITUDE OF ISOLATED ATOM ORBITAL SCATTERING FACTOR=',E
     #15.8,//)
C
      IF(JD.GT.NSL) GO TO 3000
C
      DO 2004 JF=1,NRREQ
```

TABLE E 2 . (continued)

PROGRAM FOR GENERATING CORRELATION VALUES

```
C
      RR(JF)=DELRR0+DELRR*(JF-1)
C
C
C
      GN(JF)=ANYVA2(RR(JF),R,G,CG,NR)
C
C
 2004 CONTINUE
C
C
      CALL SPLIN2(YPA,YPB,RR,GN,CG,2,2,2,NRREQ)
      GNORM=TRANS2(YPA,YPB,RR,GN,PARAM,CG,NRREQ)
      WRITE(6,3001) RR(1),RR(NRREQ),GNORM
 3001 FORMAT(//25X,'******* PAIR DISTRIBUTION FUNCTION NORMALIZATION ***
     #*****',/30X,'LOWER LIMIT OF INTEGRAL IS ',E15.8,/30X,'UPPER LIMIT O
     #F INTEGRAL IS ',E15.8,/30X,'NORMALIZATION VALUE IS ',E15.8,//)
 3000 CONTINUE
C
C
C
      DO 2003 JE=1,NFR
C
      CORSTT(JE)=DELPAV(JE,JD)
C
 2003 CONTINUE
C
C
      YPAD=(CORSTT(2)-CORSTT(1))/(RF(2)-RF(1))
C
      YBAD=0.0D0
C
```

PROGRAM FOR GENERATING CORRELATION VALUES

```
C
C
      CALL SPLIN2(YPAD,YBAD,RF,CORSTT,C,2,2,2,NFR)
C
C
C
      DO 5100 JEE=1,NRREQ
 5100 YNTG2(JEE)=GN(JEE)*ANYVA1(RR(JEE),RF,CORSTT,C,NFR)
      CALL SPLIN2(YPA,YPB,RR,YNTG2,CG2,2,2,2,NRREQ)
      CORAD=4.0D0*PI*PI*RHO*TRANS2(YPA,YPB,RR,YNTG2,PARAM,CG2,NRREQ)/FRE
     #EAT(JD)
C
C
C
      CORSTR(JD)=CORAD
C
C
C
C
      WRITE(6,2008) SCAL(JD),CORSTR(JD)
 2008 FORMAT(15X,'S= ',E15.8,10X,'CORR TO STUT FACTOR= ',E15.8)
C
 2002 CONTINUE
C
      WRITE(6,4008)
 4008 FORMAT(//25X,' ******* INVERSION OF STRUCTURE FACTOR WITH CORRECTI
     #ONS',/25X,'VALUES USED TO CORRECT THE STRUCTURE FACTOR',//)
C
      NSUX=NSU
      IF(NDELS.EQ.1)  GO TO 8001
      NSUX=1+(NSU-NSL)/NDELS
      JPM=NSL
```

TABLE E 2 (continued)

PRCGRAM FOR GENERATING CORRELATICN VALUES

```
      DO 9000 LA=1,NSUX
      SCAL(LA)=SCAL(JPM)
      CORSTR(LA)=CORSTR(JPM)
      JPM=JPM+NDELS
 9000 CONTINUE
C
 8001 CCNTINUE
      CALL SPLIN2(YPA,YPB,SCAL,CORSTR,C,2,2,2,NSUX)
      DO 4000 JJ=1,NSTRUT
      ANY1=ANYVA1(SX(JJ),SCAL,CORSTR,C,NSUX)
      WRITE(6,4001) SX(JJ),STRUT(JJ),ANY1
 4001 FORMAT(20X,'S=',E15.8,'  STRUT-1=',E15.8,'  CORR=',E15.8)
C
      YNTGND(JJ)=STRUT(JJ)-ANY1
C
      PUNCH 9500, SX(JJ),STRUT(JJ),ANY1
 9500 FORMAT(3E15.8)
 4000 CONTINUE
      WRITE(6,4004)
 4004 FORMAT(//25X,'******  RESULTS OF INVERSION OF STRUCTURE FACTOR  **
     #*****',//)
      CALL SPLIN2(YPA,YPB,SX,YNTGND,C,2,2,2,NSTRUT)
      DO 4002 JK=1,NR3
      G(JK)=TRANS2(YPA,YPB,SX,YNTGND,R(JK),C,NSTRUT)/(2.0D0*PI*PI*RHO)
      G(JK)=1.0D0+G(JK)
C
      ORD(JK)=G(JK)
      DEL=G(JK)-GL1(JK)
      WRITE(6,4003) R(JK),GL1(JK),G(JK),DEL
 4003 FORMAT(20X,'R=',E15.8,'  GEXP=',E15.8,'  GCOR=',E15.8,'  DELTA-G='
     #,E15.8)
C
 4002 CONTINUE
```

PROGRAM FOR GENERATING CORRELATICN VALUES

```
C
      CALL PLUTZ(ASS,ORD,NR3,0,2,4,1)
C
C
      DO 4500 JZ=1,NR3
 4500 ORD(JZ)=GL1(JZ)
C
      CALL PLUTZ(ASS,ORD,NR3,1,2,2,1)
C
      NR=NR3
      KEYNUM=KEYNUM+1
      IF(KEYNUM.LE.KEY) GO TO 8000
C
 1350 STOP
C
C
      END
      DOUBLE PRECISION FUNCTION ANY(RX)
      COMMCN/A1/R,G,CG,NR
      DIMENSION R(1),G(1),CG(4,1)
      ANY=ANYVA2(RX,R,G,CG,NR)
      CONTINUE
      RETURN
      END
      DOUBLE PRECISION FUNCTION YNTEG3(XR,X,C,IR)
      IMPLICIT REAL*8(A-H,O-Z)
C   THIS FUNCTION ROUTINE HAS THE JOB OF SUMMING OVER THE CCEFICIENTS         C
C   OF THE INTERPOLATED CURVE. THE INTEGRATION HAS BEEN PERFORMED ANALYTICALLY C
      DIMENSION X(1),C(4,1)
      A= C(1,IR)-C(2,IR)*X(IR) +(C(3,IR)-C(4,IR)*X(IR+1))*X(IR)*X(IR)
      B=C(2,IR)-2.DO*X(IR)*C(3,IR)+C(4,IR)*X(IR)*X(IR)+2.DO*X(IR)*X(IR+1
     X)*C(4,IR)
      D=C(3,IR)-2.DO*C(4,IR)*X(IR)-C(4,IR)*X(IR+1)
```

TABLE E 2 (continued)

PROGRAM FOR GENERATING CORRELATICN VALUES

```
      XR2=XR*XR
      YNTEG3=(A*XR2/2.D0)+B*(XR2*XR/3.D0)+D*(XR2*XR2/4.D0)+C(4,IR)*XR2*X
     #R2*XR/5.D0
 3    CONTINUE
      RETURN
      END
      DOUBLE PRECISION FUNCTION TRANS2(YPA,YPB,W,EL,R,C,NPOINT)
C   THIS FUNCTICN COMPUTES THE FOURIER SINE TRANSFORM BY FITTING THE  INPUT    C
C   TO CUBIC SPLINE CURVE PROGRAMMEC BY BRUCE KIRSTEIN.                        C
C   REMAINDER OF  PROOGRAM BY M.PILIAVIN  11 MAY, 1971     CIT E.S.            C
C   THE FORM OF THE TRANSFORM IS  ...  S F(X)*X*X*SIN(R*X)/(R*X) DX  ...       C
C   THE LIMITS FOR THE INTEGRAL  IN THE TRANSFORM ARE ZERO (LOWER)   AND       C
C   W(NPOINT)  (UPPER)    THE VALUE AT THE ABCISSA OF THE LAST INPUT POINT     C
C   YPA IS THE ESTIMATED DERIVATIVE AT THE LEFT EDGE OF THE INPUT DATA         C
C   YPB IS THE SAME AS YPA EXCEPT  AT THE RIGHT EDGE                           C
C   W  IS THE ARRAY OF POINTS ALONG THA ABCISSA                                C
C   EL IS THE ARRAY CF POINTS TO BE FOURIER TRANSFORMED                        C
C   R IS THE PARAMETER IN TRANSFORM SPACE FOR WHICH THE TRANSFORM IS DESIREC   C
C   NPOINT IS THE NUMBER OF POINTS IN THE INPUT DATA AND SHOULD BE OCD         C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION W(1),EL(1),C(4,1)
      NL1=NPCINT-1
      SUMY=C.0D0
      DO 1 JA=1,NL1
 1    SUMY=SUMY+YNTEG2(W(JA+1),W,R,C,JA)-YNTEG2(W(JA),W,R,C,JA)
      TRANS2=SUMY
      RETURN
      END
      SUBROUTINE PLUTZ(ASS,ORD,NPTS,LAB,IP,ISYS,ISP)
C
      DIMENSICN ASS(1),ORD(1),DD(3)
C
C
```

PROGRAM FOR GENERATING CORRELATICN VALUES

```
      DATA DD/3*0./
C
      CALL LABEL(0.00,0.00,0.00,ASS(NPTS),15.0,15,'SEPARATICN',10,0)
C
      IF(LAB.NE.0) GO TO 1
C
      CALL LABEL(0.00,0.00,-2.00,2.00,10.00,10,'RADIAL DISTRIBUTICN G(R)
     #',24,1)
C
 1    CONTINUE
C
      CALL PLOTXY(NPTS,ASS,ORD,ASS(1),ASS(NPTS),-2.00,2.00,LAB,IP,ISYS,I
     #SP,DD)
C
      RETURN
      END
C DATA
   31    4  120    1   14    1    0   61    0    0
 .1          3.10
G(R) FROM CATA
TEMP= 163          RHO= .78        DELR= 0.1        NR=  101
0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
0.0          0.0          0.0          0.0          0.0          0.0          -.0899       .1975
.5309        .8882        1.2341       1.5246       1.7229       1.8697       1.944        1.9362
1.89         1.8049       1.6884       1.5525       1.4141       1.284        1.163        1.0521
.9706        .9239        .8904        .87          .8599        .8543        .8504        .8535
.8598        .8679        .8777        .8892        .9013        .9155        .9296        .9455
.9604        .9768        .9891        1.0038       1.0154       1.0263       1.0373       1.047
1.0548       1.0609       1.063        1.0631       1.0603       1.057        1.0517       1.0434
1.0354       1.0258       1.0176       1.0103       1.0038       .9972        .9927        .9884
.9873        .9859        .9858        .9861        .9872        .9887        .9904        .9921
```

TABLE E 2 (continued)

```
          PRCGRAM FOR GENERATING CORRELATICN VALUES


.9945     .9968     .9986     1.0003    1.002
AR STRUCTURE FACTORS FRCM DATA        T=163 RHO=.78GM/CC
 163.     .78
-.386     -.448     -.49      -.52      -.537     -.55      -.552     -.547
-.532     -.505     -.466     -.406     -.329     -.236     -.125     .012
.169      .324      .476      .593      .658      .662      .618      .540
.425      .32       .217      .132      .063      .006      -.037     -.066
-.084     -.091     -.086     -.064     -.036     -.009     .02       .046
.069      .085      .088      .077      .05       .036      .021      .003
-.014     -.029     -.044     -.055     -.062     -.063     -.060     -.053
-.051     -.037     -.02      -.002     .014      .028      .036      .042
.046      .041      .032      .026      .017      .007      .000      -.006
-.008     -.01      -.01      -.01      -.007     -.005     .000      .008
.015      .017      .018      .016      .019      .024      .029      .028
.028      .029      .03       .032      .033      .029      .03       .03
.031      .028      .026      .026      .022      .022      .017      .019
.017      .018      .017      .02       .023      .026      .025      .023
.020      .018      .016      .014      .013      .012      .012      .013
VALUES OF 4*PI*SIN( )/LAMBDA FOR     DATA
.31       .39       .46       .54       .62       .69       .77       .85
.93       1.0       1.08      1.16      1.23      1.31      1.39      1.46
1.54      1.62      1.69      1.77      1.85      1.92      2.0       2.08
2.15      2.23      2.31      2.38      2.46      2.54      2.61      2.69
2.77      2.84      2.92      2.99      3.07      3.15      3.22      3.3
3.37      3.45      3.53      3.6       3.68      3.75      3.83      3.9
3.98      4.05      4.13      4.2       4.28      4.35      4.43      4.5
4.58      4.73      4.87      5.02      5.17      5.32      5.46      5.61
5.76      5.90      6.05      6.19      6.34      6.48      6.62      6.77
6.91      7.05      7.19      7.33      7.47      7.61      7.75      7.89
8.03      8.16      8.3       8.44      8.57      8.71      8.84      8.97
9.11      9.24      9.37      9.5       9.63      9.76      9.89      10.02
10.14     10.39     10.64     10.89     11.13     11.37     11.60     11.83
12.06     12.28     12.5      12.72     12.93     13.14     13.34     13.55
```

```
          PROGRAM FOR GENERATING CORRELATICN VALUES


13.74     13.93     14.12     14.3      14.48     14.66     14.83     15.0
CORR TO AR SCAT FACT AVED ORIENTS AND SUMD  OVER ORBS,R= 0.40000000E 01
R= 4.0000000 AU  NUMEX=  14 DELTA-X= 0.0264585 1/A.U
 VALUES OF DELTA-F --SUBSCRIPT P
 0.0       0.1179545 0.0947216-0.1897002-0.0940612 0.0557453 0.1332054 0.0040942
-0.0452736 0.0192874 0.0498453 0.0189602-0.0020680-0.0010312
CORR TO AR SCAT FACT AVED ORIENTS AND SUMD  OVER ORBS,R= 0.74000000E 01
R= 7.4000000 AU  NUMEX=  14 DELTA-X= 0.0264585 1/A.U
 VALUES OF DELTA-F --SUBSCRIPT P
0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
CORR TO AR SCAT FACT AVED ORIENTS AND SUMD  OVER ORBS,R= 0.75000000E 01
R= 7.5000000 AU  NUMEX=  14 DELTA-X= 0.0264585 1/A.U
 VALUES OF DELTA-F --SUBSCRIPT P
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0
CORR TO AR SCAT FACT AVED ORIENTS AND SUMD  OVER ORBS,R= 1.50000000E 01
R=15.0000000 AU  NUMEX=  14 DELTA-X= 0.0264585 1/A.U
 VALUES OF DELTA-F --SUBSCRIPT P
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0
SCATTERING FACTORS FOR ISOLATED AR ATOMS--GILBERT WAHL WF R=7.5 AU
 18.0     17.567    16.4062   14.8403   13.1982   11.7018   10.4515   9.4608
8.6962    8.1067    7.6407    7.2544    6.9149    6.5998
```

TABLE E 2 (continued)

PROGRAM FOR GENERATING CORRELATION VALUES

```
      SUBROUTINE SPLIN2(YPA,YPB,X,Y,C,NPRINT,NSTRA1,NSTRA2,NPOINT)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION X(1),Y(1),C(4,1)
      DIMENSION B(600),A(3,600),YP(600),DELTAX(600)
C    VALUES OF YPA,YPB,NPRINT,NSRA1,NSTRA1 MUST BE SUPPLIED   IN THE CALLING    C
C    PROGRAM OR SUBROUTINE IN THE ARGUMENT OF SPLINE.                           C
C    THE INTERPOLATED VALUES OF Y ARE GIVEN IN THE FUNCTION F, WHICH MUST BE    C
C    DECLARED EXTERNAL F IN THE PROGRAM USING IT. THE FUNCTION TO BE INTER-     C
C    POLATED MUST BE PUT IN COMMON/CUBIK/, AS WELL AS THE INDEPENDENT           C
C    VARIABLE.   CUBIK MUST BE PRESENT IN FUNCTION F AS WELL AS THE PROGRAM     C
C      NSTRA1=1 MEANS STRAIGHT-LINE FIT BETWEEN POINTS 1 AND 2.
C      NSTRA1=2 MEANS USE SPLINE BETWEEN POINTS 1 AND 2.
C      NSTRA2=1 MEANS STRAIGHT-LINE FIT BETWEEN POINTS NPOINT-1 AND NPOINT.
C      NSTRA2=2 MEANS USE SPLINE BETWEEN POINTS NPOINT-1 AND NPOINT.
C      X AND Y ARE THE GIVEN POINTS FOR INTERPOLATING.
C      XT ARE THE VALUES OF X FOR WHICH INTERPOLATED Y-VALUES ARE DESIRED.
C      THE XT VALUES CAN BE IN ANY ORDER.
C      YPA=GIVEN DERIVATIVE AT LEFT EDGE.
C      YPB=GIVEN DERIVATIVE AT RIGHT EDGE.
C      N=NUMBER OF INTERVALS=NUMBER OF GIVEN DATA POINTS MINUS ONE.
C      NPOINT = NUMBER OF GIVEN POINTS.
C      NPRINT=1, PRINT EVERYTHING.
C      NPRINT=2, OMIT PRINTING.
C
      N=NPOINT-1
      N1=N-1
      N2=N-2
      DO 310 J=1,N
      DELTAX(J)=X(J+1)-X(J)
310   CONTINUE
      GO TO (500,501), NPRINT
500   WRITE (6,71) X(1),X(NPOINT),N
71    FORMAT(1H1,10X,'INTERPOLATING BETWEEN X = ',1PE11.4,' AND X = ',1P
```

PROGRAM FOR GENERATING CORRELATION VALUES

```
     XE11.4,' WITH ',I5,' INTERVALS.')
      WRITE (6,69)
69    FORMAT(/,10X,'USING   C U B I C   S P L I N E   ****************')
      WRITE (6,314) YPA,YPB
314   FORMAT(/,10X,'DERIVATIVES AT THE ENDS ARE ',1PE11.4,' AND ',1PE11.
     X4)
C
C     SOLVING FOR N-1 UNKNOWNS.
C     MESH POINTS ARE NUMBERED: 1,2,3, . . . ;  NOT  0,1,2,3 . . .
C     AT MESH POINT 1 IS YPA FOR THE DERIVATIVE, X(1), AND Y(1).
C     AT MESH POINT 2 IS YP(1) FOR THE DERIVATIVE, X(2) AND Y(2).
C     ETC.
C     THERE ARE N+1 VALUES OF Y AT THE MESH POINTS.
C     Y(J+1)=Y AT MESH POINT J.
C
C     FILL MATRIX.
C
501   DO 440 J=1,N1
      R=DELTAX(J+1)/DELTAX(J)
      B(J)=3.0 D0*(R*(Y(J+1)-Y(J))+(Y(J+2)-Y(J+1))/R)
440   CONTINUE
      B(1)=B(1)-DELTAX(2)*YPA
      B(N-1)=B(N-1)-DELTAX(N)*YPB
C
C     FILL DIAGONAL ELEMENTS
C
      DO 460 J=1,N1
      A(2,J)=2.0 D0*(DELTAX(J+1)+DELTAX(J))
460   CONTINUE
      DO 470 J=1,N2
      A(1,J)=DELTAX(J)
      A(3,J)=DELTAX(J+2)
470   CONTINUE
```

TABLE E 2 (continued)

PROGRAM FOR GENERATING CORRELATICN VALUES

```
C
C     REDUCE TRIDIAGCNAL MATRIX.
C
      DO 480 J=1,N2
C
C     NORMALIZE THE ROW BY THE PIVOT ELEMENT, THIS PUTS UNITY ON THE DIAGCNAL.
C
      A(1,J)=A(1,J)/A(2,J)
      B(J)=B(J)/A(2,J)
C
C     SUBTRACT FROM SECCND ROW.
C     NOTE THAT THE SYSTEM IS NOT REDUCED THROUGH THE LAST ROW.
C
      A(2,J+1)=A(2,J+1)-A(1,J)*A(3,J)
      B(J+1)=B(J+1)-B(J)*A(3,J)
480   CCNTINUE
C
C     BEGIN BACK SUBSTITUTION, NOTE THAT THE DIAGCNAL IS UNITY.
C
      YP(N-1)=B(N-1)/A(2,N-1)
      DO 490 J=1,N2
      K=N-1-J
      YP(K)=B(K)-YP(K+1)*A(1,K)
490   CCNTINUE
      GO TO (303,304), NPRINT
303   WRITE (6,599)
599   FORMAT(///,10X,'MESH POINT,    X,    ESTIMATED DERIVATIVE',/)
      DO 6C0 K=1,N1
      WRITE (6,601) K,X(K+1),YP(K)
601   FCRMAT(10X,I4,2(5X,1PE11.4))
600   CONTINUE
C
C     CALCULATE COEFFICIENTS FOR EACH INTERVAL.
```

```
          PROGRAM FOR GENERATING CORRELATICN VALUES


C
      WRITE (6,701)
701   FORMAT(1H1,10X,'THE COEFFICIENTS FOR EACH INTERVAL:  X(J-1) ) X )
     XX(J)',/,10X,'Y = C(1,J) + C(2,J)*(X-X(J-1)) + (X-X(J-1))**2*(C(3,J
     X) + C(4,J)*(X-X(J)))')
      WRITE (6,7C2)
702   FORMAT(/,10X,'INTERVAL          C(1,J)          C(2,J)          C(3
     X,J)          C(4,J)',/)
304   C(1,1)=Y(1)
      C(2,1)=YPA
      D2=DELTAX(1)**2
      C(3,1)=(Y(2)-Y(1)-YPA*DELTAX(1))/D2
      C(4,1)=(YP(1)-C(2,1)-2.0 DO*C(3,1)*DELTAX(1))/D2
      DO 7C0 J=2,N1
      C(1,J)=Y(J)
      C(2,J)=YP(J-1)
      D2=DELTAX(J)**2
      C(3,J)=(Y(J+1)-Y(J)-YP(J-1)*DELTAX(J))/D2
      C(4,J)=(YP(J)-C(2,J)-2.0 DO*C(3,J)*DELTAX(J))/D2
700   CONTINUE
      C(1,N)=Y(N)
      C(2,N)=YP(N-1)
      D2=DELTAX(N)**2
      C(3,N)=(Y(N+1)-Y(N)-YP(N-1)*DELTAX(N))/D2
      C(4,N)=(YPB-C(2,N)-2.0 DO*C(3,N)*DELTAX(N))/D2
      GO TO (210,219), NPRINT
210   DC 215 J=1,N
      WRITE (6,699) J,(C(I,J),I=1,4)
699   FORMAT(13X,I4,3X,4(5X,1PE11.4))
215   CCNTINUE
C
C     USING STRAIGHT LINE APPROXIMATICN IN INTERVAL =1.
C     Y = M*(X-X(1)) + B    FOR X(1) ) X ) X(2).
```

TABLE E 2 (continued)

PROGRAM FOR GENERATING CORRELATION VALUES

```
C
219    GO TO (220,221), NSTRA1
220    C(1,1)=Y(1)
       C(2,1)=(Y(2)-Y(1))/DELTAX(1)
       C(3,1)=0.D0
       C(4,1)=0.D0
       IF(NPRINT.EQ.1) WRITE (6,670) C(1,1),C(2,1)
670    FORMAT(//,10X,'IN INTERVAL =1, USE STRAIGHT LINE:  Y = M*(X-X(1))
      X+ B FOR X(1) ) X ) X(2)',/,10X,' WITH M = ',1PE11.4,' AND B = ',1P
      XE11.4)
C
C      USE STRAIGHT LINE FIT FOR LAST INTERVAL.
C      Y = M*(X - X(N)) + B     FOR    X(N) ) X ) X(NPOINT).
C
221    GO TO (222,223), NSTRA2
222    C(1,N)=Y(N)
       C(2,N)=(Y(NPOINT)-Y(N))/DELTAX(N)
       C(3,N)=0.D0
       C(4,N)=0.D0
       IF(NPRINT.EQ.1) WRITE (6,225) C(1,N),C(2,N)
225    FORMAT(//,10X,'IN INTERVAL N, THE LAST ONE, USE STRAIGHT LINE:  Y
      X= M*(X-X(N)) + B  FOR X(N) ) X ) X(NPOINT)',/,10X,'WHERE M = ',1PE
      X11.4,' AND M = ',1PE11.4)
C
 223   CONTINUE
       RETURN
       END
       DOUBLE PRECISION FUNCTION TRANS2(YPA,YPB,W,EL,R,C,NPOINT)
C    THIS FUNCTION COMPUTES THE FOURIER SINE TRANSFORM BY FITTING THE  INPUT    C
C    TO CUBIC SPLINE CURVE PROGRAMMED BY BRUCE KIRSTEIN.                        C
C    REMAINDER OF  PROOGRAM BY M.PILIAVIN  11 MAY, 1971     CIT E.S.            C
C    THE FORM OF THE TRANSFORM IS  ...  S F(X)*X*X*SIN(R*X)/(R*X) DX  ...       C
C    W  IS THE ARRAY OF POINTS ALONG THA ABCISSA                                C
```

PROGRAM FOR GENERATING CORRELATION VALUES

```
C    THE LIMITS FOR THE INTEGRAL  IN THE TRANSFORM ARE ZERO (LOWER)   AND       C
C    W(NPOINT)  (UPPER)    THE VALUE AT THE ABCISSA OF THE LAST INPUT POINT     C
C    YPA IS THE ESTIMATED DERIVATIVE AT THE LEFT EDGE OF THE INPUT DATA         C
C    YPB IS THE SAME AS YPA EXCEPT  AT THE RIGHT EDGE                           C
C    EL IS THE ARRAY OF POINTS TO BE FOURIER TRANSFORMED                        C
C    R IS THE PARAMETER IN TRANSFORM SPACE FOR WHICH THE TRANSFORM IS DESIRED   C
C    NPOINT IS THE NUMBER OF POINTS IN THE INPUT DATA AND SHOULD BE ODD         C
       IMPLICIT REAL*8(A-H,O-Z)
       DIMENSION W(1),EL(1),C(4,1)
       NL1=NPOINT-1
       CALL SPLIN2(YPA,YPB,W,EL,C,2,2,2,NPOINT)
       SUMY=0.0D0
       DO 1 JA=1,NL1
 1     SUMY=SUMY+YNTEG2(W(JA+1),W,R,C,JA)-YNTEG2(W(JA),W,R,C,JA)
       TRANS2=SUMY
       RETURN
       END
       DOUBLE PRECISION FUNCTION YNTEG2(XR,X,S,C,IR)
       IMPLICIT REAL*8(A-H,O-Z)
C    THIS FUNCTION ROUTINE HAS THE JOB OF SUMMING OVER THE COEFICIENTS          C
C    OF THE INTERPOLATED CURVE. THE INTEGRATION HAS BEEN PERFORMED ANALYTICALLY C
       DIMENSION X(1),C(4,1)
       A= C(1,IR)-C(2,IR)*X(IR) +(C(3,IR)-C(4,IR)*X(IR+1))*X(IR)*X(IR)
       B=C(2,IR)-2.D0*X(IR)*C(3,IR)+C(4,IR)*X(IR)*X(IR)+2.D0*X(IR)*X(IR+1
      X)*C(4,IR)
       D=C(3,IR)-2.D0*C(4,IR)*X(IR)-C(4,IR)*X(IR+1)
       TH=XR*S
       TH2=TH*TH
       TH3=TH*TH2
       SI=DSIN(TH)
       CO=DCOS(TH)
       S3=S*S*S
       S4=S3*S
```

TABLE E 2 (continued)

PROGRAM FOR GENERATING CORRELATION VALUES

```
      S5=S4*S
      IF(S.LT.1.0D-4) GO TO 2
      A1=A*(SI-TH*CO)/S3
      B1=B*(TH*SI+TH*S3*((SI-TH*CO)/S3)+2.D0*CO)/S4
      D1=D*(2.D0*TH2*SI+(TH2-6.D0)*S3*((SI-TH*CO)/S3))/S5
      SC=C(4,IR)*(3.D0*TH3*SI+TH3*S3*((SI-TH*CO)/S3)-12.D0*((TH*SI+TH*S3
     X*((SI-TH*CO )/S3)+2.D0*CO)/S4)*S4)/(S3*S3)
      YNTEG2=A1+B1+D1+SC
      GO TO 3
 2    CONTINUE
      XR3=XR*XR*XR
      YNTEG2=(A*XR3/3.D0)+B*(XR3*XR/4.D0)+D*(XR3*XR*XR/5.D0)+C(4,IR)*XR3
     #*XR3/6.D0
 3    CONTINUE
      RETURN
      END
      DOUBLE PRECISION FUNCTION ANYVA2(RX,X,Y,C,NPOINT)
      IMPLICIT REAL*8(A-H,O-Z)
C    PROGRAM TO COMPUTE THE VALUE OF ANY FUNCTION FITTED TO CUBIC SPLINE        C
C    THIS FUNCTION USES RESULTS OF SUBROUTINE SPLINE WHOSE CALL PRECEDES IT     C
C    RX IS THE POINT AT WHICH THE FUNCTION IS TO BE INTERPOLATED                C
C    X  IS THE ARRAY OF INDEPENDENT VARIABLES WHICH DESCRIBES THE LOCATION      C
C    OF THE DEPENDENT VARIABLE Y  FITTED TO THE CUBIC SPLINE CURVE              C
C    WHICH GEBERATES OR READS IN THE VALUES OF Y,X USED FOR INTERPOLATING.    C
      DIMENSION X(1),Y(1),C(4,1)
      DO 815 K=2,NPOINT
      IF(RX.LE.X(K).AND.RX.GE.X(K-1)) GO TO 807
 815  CONTINUE
      WRITE(6,816) RX
 816  FORMAT(//,10X,'*******   RX= ',1PE11.4,'IS NOT IN THE INTERPOLATED
     +RANGE.    *********')
      GO TO 810
 807  K=K-1
```

PROGRAM FOR GENERATING CORRELATION VALUES

```
      XX=RX-X(K)
      ANYVA2= C(1,K)+C(2,K)*XX+XX*XX*(C(3,K)+C(4,K)*(RX-X(K+1)))
 810  CONTINUE
      RETURN
      END
      SUBROUTINE ANYXFM(X,Y,XREQ,YREQ,CONST,ORD,NP,NPREQ,KEYXFM)
      IMPLICIT REAL*8(A-H,O-Z)
C
C
C    KEYXFM=1 DOES G(R); =2 DOES C(R)
C
C
C
      REAL*4 ORD(1)
C
      DIMENSION X(1),Y(1),XREQ(1),YREQ(1),C(4,201)
C

C
      YPA=0.0D0
      YPB=0.0D0
C
C
C
      CALL SPLIN2(YPA,YPB,X,Y,C,2,2,2,NP)
C
      GO TO (3,4),KEYXFM
C
C
 3    CONTINUE
C
C
C
```

TABLE E 2 (continued)

PROGRAM FOR GENERATING CORRELATION VALUES

```
      DO 1 J=1,NPREQ
C
      YREQ(J)=TRANS2(YPA,YPB,X,Y,XREQ(J),C,NP)*CONST+1.0D0
      ORD(J)=YREQ(J)
C
C
C
C
 1    CONTINUE
C
      GO TO 5
C
C
C
C
 4    CONTINUE
C
      DO 6 JA=1,NPREQ
      YREQ(JA)=TRANS2(YPA,YPB,X,Y,XREQ(JA),C,NP)*CONST
      ORD(JA)=YREQ(JA)
C
 6    CONTINUE
C
 5    CONTINUE
C
      RETURN
C
C
      END
```

TABLE E 3
PROGRAM FCR CCMPARING RESULTS

```
C
C    PROGRAM TO COMPUTE RDF AND C(R) AND U(R) WITH AND WITHOUT CORRECTIONS     C
C    TO THE SCATTERED INTENSITY I(S)                                           C
C    KTYPE=1 PLOTS G(R)
C    KTYPE=2 PLOTS C(R)
C    KTYPE=3 PLOTS U(R)
C    KTYPE=4 PLOTS CORRECTIONS TO I(S)
C    KEYXFM=1 DOES G(R) TRANSFORMS
C    KEYXFM=2 DOES C(R) TRANSFORMS
C
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*4 ASS(151),ORD(151),ORDC(151),TOP
      DIMENSION COR1(101),COR2(101),U(101)
      DIMENSION TITL2(10),TITLE(10),COR(101),CRL(101),CRLC(101)
      DIMENSION X(201),Y(201),XREQ(201),YREQ(201),YREQ2(201),PERG(201)
C
      COMMCN/A/TOP
C
C
      REAC(5,1) NP,NCOR,NPREQ,NPUN
 1    FORMAT(4I5)
      READ(5,2) TITL2
C
      READ(5,2) TITLE
 2    FORMAT(10A8)
C
      READ(5,3) TEMP,RHO
 3    FORMAT(2E15.8)
C
C
      RHO=RHC*(.2703D0)/18.D0



          PROGRAM FCR CCMPARING RESULTS


C
      DC 5 J=1,NP
      READ(5,4) X(J),Y(J),COR(J)
 4    FCRMAT(3E15.8)
C
      COR(J)=-COR(J)
C
C
C
      ASS(J)=X(J)
C
      ORD(J)=CCR(J)
C
      ORDC(J)=Y(J)
      CRL(J)=Y(J)/(1.0D0+Y(J))
      CRLC(J)=(Y(J)+CCR(J))/(1.0D0+Y(J)+CCR(J))
      WRITE(6,6) X(J),Y(J),COR(J),CRL(J),CRLC(J)
 6    FORMAT('S=',E16.8,'I= ',E16.8,'COR=',E16.8,'Y/1+Y=',E16.8,'CRLC=',
     #E16.8)
C
C
 5    CONTINUE
C
 1000 CCNTINUE
C
C
      PI=3.14159265359D0
      CONST=1.0D0/(2.0D0*PI*PI*RHO)
C
C
C
      TOP=.02
      CALL IPLOT(ASS,ORD,NP,0,2,2,4)
```

TABLE E 3 (continued)

PROGRAM FCR CCMPARING RESULTS

```
C
      CALL ANYXFM(X,Y,XREQ,YREQ,CONST,CRD,NP,NPREC,KEYXFM)
C
C
      DO 1001 J=1,3
      IF(DABS(YREQ(J)).GE.2.0D0) YREQ(J)=-1.0D0
 1001 CONTINUE
C
      CALL GPLOT(ASS,ORD,NPREQ,0,1,2,1)
C
C
C
C
C
C   COMPUTE AND PLOT TRANSFCRM OF CORRECTICNS ALCNE
C
      CALL ANYXFM(X,COR,XREQ,YREQ2,CCNST,ORD,NP,NPREQ,2)
C
C
      CALL GPLOT(ASS,ORD,NPREQ,0,2,2,4)
C
C
C   COMPUTE G(R) WITH CORRECTIONS
      DO 9 JF=1,NPREQ
      YREQ2(JF)=YREQ2(JF)+YREQ(JF)
      ORD(JF)=YREQ2(JF)
  9   CCNTINUE
C
C
C
C
      CALL GPLOT(ASS,ORD,NPREQ,1,2,4,4)
C
```

PROGRAM FCR CCMPARING RESULTS

```
C
      TOP=1.0
      CALL IPLOT(ASS,ORDD,NP,1,1,2,1)
C
C
      DO 10 JE=1,NPREC
      XREQ(JE)=0.1D0*(JE-1)
      ASS(JE)=XREQ(JE)
 10   CONTINUE
C
C   COMPUTE C(R) WITHOUT CORRECTICNS
      KEYXFM=2
      CALL ANYXFM(X,CRL,XREQ,COR1,CONST,ORD,NP,NPREQ,KEYXFM)
C
      DO 1002 J=1,3
      IF(DABS(COR1(J)).GE.12.0D0) COR1(J)=-10.0D0
 1002 CONTINUE
C
      CALL CPLOT(ASS,ORD,NPREQ,0,1,2,1)

C
C   COMPUTE C(R) WITH CORRECTIONA
      CALL ANYXFM(X,CRLC,XREQ,COR2,CONST,CRD,NP,NPREQ,KEYXFM)
C
C
      DO 1003 J=1,3
      IF(DABS(COR2(J)).GE.12.0D0) COR2(J)=-10.0D0
 1003 CONTINUE
      CALL CPLCT(ASS,ORD,NPREQ,1,2,2,4)
C
C
      KEYXFM=1
C   COMPUTE G(R)
```

TABLE E 3 (continued)

PROGRAM FCR CCMPARING RESULTS

```
C   COMPUTE THE ENRGY WITHOUT CORRECTICNS
      NPRECL=32
      CALL ENERGY(COR1,YREQ,TEMP,U,CRD,NPRECL,NPREQ)
      CALL EPLOT(ASS,ORD,NPREQL,NPREQ,0,1,2,1)
C
C   COMPUTE THE ENERGY WITH CORRECTICNS
      CALL ENERGY(COR2,YREQ2,TEMP,U,ORD,NPREQL,NPREQ)
C
      CALL EPLCT(ASS,CRD,NPREQL,NPREQ,1,2,4,4)
C
C
      DO 12 KA=1,NPREG
      PERG(KA)=C.ODO
      IF(CABS(YREQ(KA)).GE.1.0D-6) PERG(KA)=100.D0*(YREQ2(KA)-YREG(KA))/
     #YREG(KA)
C
C
 12   CCNTINUE
C
C   COMPUTE PERCENTAGES DEVIATIONS IN C(R) AND G(R) RELATIVE TO UNCORRECTEC VALS
C
C
      WRITE(6,100)  TEMP,RHO
 100  FORMAT(1H1/30X,'>>>>>>    RESULTS OF TRANSFORMATICNS FOR AR      <<
     #<<<<',//10X,'TEMP= ',E15.8,' KELVIN',10X,'RHC= ',E15.8,'  ATCMS/A*
     #*3',////,'       R=          ',' RDF NO INTERACTS',' RDF    INTERACT
     #S',' PERCENT DEVIATION',' C(R) NO INTERACTS',' C(R)    INTERACTS',
     #' PERCENT DEVIATICN',///)
C
      DO 30 NM=1,NPREG
      WRITE(6,101)  XREC(NM),YREQ(NM),YREQ2(NM),PERG(NM),CCR1(NM),COR2(N
     #M)
 101  FCRMAT(6(E15.8,2X))
```

PRCGRAM FCR COMPARING RESULTS

```
 30   CONTINUE
C
C
C
C
C
C
C
      STOP
C
      END
      SUBROUTINE GPLOT(ASS,ORD,NPTS,LAB,IP,ISYS,ISP)
      DIMENSION ASS(1),ORD(1),DD(3),FMT(2),XOUT(5),OUT(5)
      DATA DD/3*0.0/
      DATA XOUT/2.00,2.00,11.00,11.00,2.00/,OUT/1.500,7.50,7.50,1.5,1.5/
C
      IF(LAB.EQ.0) GO TO 1
C
      CALL PLOTXY(5,XOUT,OUT,0.,15.,0.,10.,0,1,2,2,DD)
C
      CALL LABEL(4.0,3.0,0.0000,9.CC00000,6.0,6,'R     A',6,0)
C
      CALL LABEL(4.0,3.0,-3.00,3.00,4.0,4,'G(R)',4,1)
C
      CALL SYSSYM(4.0,2.35,.1,'FIG.        RADIAL CISTRIBUTICN FUNCTICNS
     #FROM AR X-RAY DATA.',60,0.)
C
      CALL SYSSYM(4.2,2.20,.1,'    UNCORRELATED SCATTERING',27,0.)
      CALL SYSSYM(7.25,2.20,.10,'      CORRELATED SCATTERING',27,0.)
C
      CALL SYSSYM(4.20,2.05,.10,'    DEVIATION DUE TO CCRRELATICN',32,0.
     #0)
 1    CCNTINUE
```

TABLE E 3 (continued)

```
            PRCGRAM FCR CCMPARING RESULTS


       CALL FLOTXY(NPTS,ASS,ORD,-6.000,16.500000,-7.50,7.50,LAB,IP,ISYS,I
      #SP,DD)
       RETURN
       END
       SUBROCTINE IPLOT(ASS,ORD,NPTS,LAB,IP,ISYS,ISP)
       COMMCN/A/TOP
       DIMENSICN ASS(1),ORC(1),DD(3),FMT(2),XOUT(5),OUT(5)
       DATA CD/3*0.0/,FMT/'(F7.','3)'/
       DATA XOUT/2.00,2.00,11.00,11.00,2.00/,OUT/1.500,7.50,7.50,1.5,1.5/
C
       IF(LAB.EG.0) GO TO 1
C
       CALL FLOTXY(5,XCUT,OUT,0.,15.,0.,10.,0,1,2,2,DD)
C
       CALL LABEL(4.0,3.0,0.0000,9.CC00000,6.0,6,'S  1/A',6,0)
C
       CALL LABEL(4.0,3.0,-1.00,1.00,4.0,4,'STRUCTURE FACTOR',16,1)
C
        CALL LABEL(3.1,3.0,-.01,.01,4.0,-4,' ',1,1)
       CALL SYSSYM(2.8,3.55,.16,'CORRELATION INTENSITY',21,90.0)
C
       DC 100 J=1,5
       TOPO=(.02*(J-3)/2)
       YB=2.70+1.0*(J-1)
       CALL PRTNUM(3.0,YB,.12,TOPO,FMT,90.0)
 100   CONTINUE
C
C
C
       CALL SYSSYM(4.0,2.35,.1,'FIG.             STRUCTURE FACTOR FRCM AR
      #X-RAY CATA',51,0.)
C
       CALL SYSSYM(4.0,2.20,.1,'                 CORRECTICN DUE TO CORRELA
```

```
            PRCGRAM FCR CCMPARING RESULTS


      #TION',45,0.)
C
 1     CONTINUE
       TPPP=2.50*TOP
       CALL PLOTXY(NPTS,ASS,ORD,-6.000,16.500000,-TPPP,TPPP,LAB,IP,ISYS,I
      #SP,DC)
       RETURN
       END
       SUBROUTINE CPLCT(ASS,ORD,NPTS,LAB,IP,ISYS,ISP)
       DIMENSION ASS(1),ORC(1),UD(3),FMT(2),XOUT(5),OUT(5)
       DATA CD/3*0.0/,FMT/'(F6.','2)'/
       DATA XOUT/2.00,2.00,11.00,11.00,2.00/,OUT/1.500,7.50,7.50,1.5,1.5/
C
       IF(LAB.EQ.0) GO TC 1
C
       CALL PLOTXY(5,XCUT,OUT,U.,15.,0.,10.,0,1,2,2,DD)
C
       CALL LABEL(4.0,3.0,0.0000,9.C000000,6.0,6,'R    A',6,0)
C
       CALL LABEL(4.0,3.0,-10.0,10.0,4.0,-4,' ',1,1)
C
       CALL SYSSYM(3.70,4.80,.16,'C(R)',4,90.0)
C
       DO 100 J=1,5
       TOPO=12.0*(J-3)/2
       YB=2.65+1.0*(J-1)
       CALL PRTNUM(3.9,YB,.12,TOPO,FMT,90.0)
 100   CONTINUE
C
       CALL SYSSYM(4.0,2.35,.1,'FIG.        DIRECT CORRELATICN FUNCTICNS
      #FRCM AR X-RAY CATA.',60,0.)
C
       CALL SYSSYM(4.2,2.20,.1,'    UNCORRELATED SCATTERING',27,0.)
```

TABLE E 3 (continued)

```
    PROGRAM FCR CCMPARING RESULTS


      CALL SYSSYM(7.25,2.20,.10,'       CORRELATED SCATTERING',27,0.)
C
 1    CCNTINUE
      CALL PLOTXY(NPTS,ASS,ORD,-6.000,16.500000,-30.0,30.0,LAB,IP,ISYS,I
     #SP,DC)
      RETUFN
      END
      SUBRCUTINE EPLCT(ASS,ORD,NPRECL,NPRECU,LAB,IP,ISYS,ISP)
      DIMENSIGN ASS(1),ORD(1),DD(3),FMT(2),XOUT(5),OUT(5)
      DIMENSION AST(101),ORT(101)
      CATA CC/3*0.0/
      DATA XOUT/2.00,2.00,11.00,11.00,2.00/,CUT/1.50C,7.50,7.50,1.5,1.5/
      DATA FMT/'(F6.','1)'/
C
      NUF=NPRECU-NPRECL+1
      DO 2 JB=1,NUP
      AST(JB)=ASS(NPRECL+JB-1)
      ORT(JB)=ORD(NPRECL+JB-1)
 2    CONTINUE
      IF(LAB.EQ.0) GO TO 1
C
      CALL PLOTXY(5,XOUT,OUT,0.,15.,0.,10.,0,1,2,2,DD)
C
      CALL LABEL(4.0,3.0,0.0000,9.C000000,6.0,6,'R     A',6,0)
C
      CALL LABEL(4.0,3.0,-200.,200.,4.0,-4,' ',1,1)
C
      CALL SYSSYM(3.70,4.55,.16,'U(R)/K',6,90.0)
C
C
      DO 1CC J=1,5
      TOPO=(200.0*(J-3)/2)
      YB=2.60+1.0*(J-1)
```

```
    PROGRAM FCR COMPARING RESULTS


      CALL PRTNUM(3.90,YB,.12,TOPO,FMT,90.)
100   CCNTINUE
      CALL SYSSYM(4.0,2.35,.1,'FIG.       INTERMOLECULAR ENERGY FOR ARGO
     #N FRCM X-RAY CATA (PY THEORY).',71,0.0)
C
      CALL SYSSYM(4.2,2.20,.1,'    UNCORRELATED SCATTERING',27,0.)
      CALL SYSSYM(7.25,2.20,.10,'       CORRELATED SCATTERING',27,0.)
C
 1    CONTINUE
      NPTS=NUP
      CALL PLOTXY(NPTS,AST,ORT,-6.000,16.500000,-500.,500.,LAB,IP,ISYS,I
     #SP,DD)
      RETUFN
      END
      SUBRCUTINE ENERGY(C,G,T,U,ORD,NPREQL,NPRECU)
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*4 ORD(1)
      DIMENSION C(1),G(1),U(1)
      WRITE(6,3) T
 3    FCRMAT(//20X,' PERCUS-YEVICK ENERGIES FCR ARGON  T= ',E15.8,//)
      DO 1 JA=NPREQL,NPREQU
C
      U(JA)=300.000
      IF(DABS(G(JA)).GE.1.0D-6) YEP=C(JA)/G(JA)
C
      IF(YEP.LE.1.000) U(JA)=T*DLOG(1.0D0-YEP)
      R=.1000*(JA-1)
      ORD(JA)=U(JA)
      WRITE(6,2) R,U(JA)
 2    FORMAT(5X,'R= ',E15.8,10X,'U/K= ',E15.8)
 1    CCNTINUE
      RETURN
      END
```