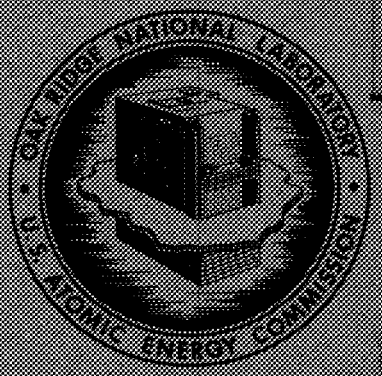
cy. 3

ORNL-4578
UC-4 – Chemistry

X-RAY DIFFRACTION DATA ON LIQUID WATER IN THE TEMPERATURE RANGE 4°C – 200°C

A. H. Narten



OAK RIDGE NATIONAL LABORATORY
operated by
UNION CARBIDE CORPORATION
for the
U. S. ATOMIC ENERGY COMMISSION

Printed in the United States of America. Available from Clearinghouse for Federal Scientific and Technical Information, National Bureau of Standards, U.S. Department of Commerce, Springfield, Virginia 22151
Price: Printed Copy $3.00; Microfiche $0.65

ORNL-4578

Contract No. W-7405-eng-26

CHEMISTRY DIVISION

X-RAY DIFFRACTION DATA ON LIQUID WATER IN THE TEMPERATURE RANGE 4°C - 200°C

A. H. Narten

JULY 1970

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee
operated by
UNION CARBIDE CORPORATION
for the
U.S. ATOMIC ENERGY COMMISSION

CONTENTS

ABSTRACT

This report describes x-ray diffraction data on liquid water at eight temperatures between $4^{o}C$ and $200^{o}C$, and on heavy water at one temperature ($4^{o}C$). Except for one new data set ($20^{o}C$), the intensity and correlation functions were derived from the tabulated raw data reported previously (ORNL-3997). Unlike the earlier intensity and radial distribution functions, the present ones were derived using more accurate values for the atomic scattering amplitudes, and results from small angle x-ray scattering were included.

The hydrogen bonds in liquid water form an extensive three-dimensional network, and over short distances from any origin the average deviation from ideal tetrahedral coordination is quite small. However, continuous small variations in instantaneous local environments result in the loss of all positional correlation between molecules a few molecular radii away from any starting point. There is, near the melting point, evidence for preferred average orientation between pairs of neighboring water molecules, but at $200^{o}C$ water molecules are "seen" by x-rays as randomly oriented.

1. INTRODUCTION

The first x-ray diffraction patterns from liquid water were obtained by Meyer[1] (1930), Stewart[2] (1931), and Amaldi[3] (1931). Katzoff[4] (1934) was the first to apply to water the method of Fourier analysis. Morgan and Warren[5] (1938) measured and analyzed the x-ray scattering from liquid water at five temperatures between the melting and boiling points. Between 1938 and 1962 various x-ray studies of water have been reported;[6-10] these studies have not added to Morgan and Warren's results. The most extensive study of water by x-ray diffraction has been carried out at Oak Ridge National Laboratory;[11-15] this work, started in 1961 and still continuing, has considerably improved and extended upon Morgan and Warren's[5] classical study both in resolution and temperature range.

Small-angle scattering data on water have been reported by a number of authors,[15-19] all work being in good agreement. The very accurate results of Levelut and Guinier,[18] Chonacky and Beeman,[19] and Hendricks[15] do not differ significantly from each other.

All published large-angle x-ray work on water, although of varying quality, is in essential agreement. An apparent discrepancy between one set of results[9,10] and those of other workers seems now resolved[20] as due to differences in the presentation and interpretation of the data. With the exception of the Oak Ridge work,[11-14] approximations and

assumptions were made in the reduction and presentation of all published large-angle x-ray data on water, and this makes the detailed comparison of different studies difficult. The following discussion is based exclusively on the Oak Ridge data, and these results will be compared only with Morgan and Warren's work. Although Morgan and Warren[5] in their data reduction make the assumption that "since the scattering by hydrogen is almost completely Compton modified radiation, it is justified to treat water as a one-atom substance," their presentation is sufficiently detailed to make such a comparison meaningful.

2. DATA COLLECTION AND REDUCTION

Except for one new data set (20°C), the intensity and radiation distribution functions presented in this report were derived from the tabulated raw data (Section 3.1 of Ref. 12) previously reported. Unlike the earlier intensity and correlation functions,[11,13,14] the present curves were derived using more accurate values for the atomic scattering amplitudes and results from small-angle x-ray scattering were included.

The small-angle scattering experiments will be described elsewhere.[15] Only a short outline of the large-angle measurements will be given in this section and some details of particular importance in the case of water will be discussed.

2.1 Diffractometer. The measurements were made with a diffractometer specially designed for the study of liquid samples, described in detail elsewhere.[21] Use is made of a divergent-beam technique similar to the Bragg-Brentano system used for powder samples. Monochromatic radiation (MoK_α) is obtained through the use of a bent and ground crystal monochromator mounted in the diffracted beam. This geometry and slit arrangement[21] completely eliminates sample holder absorption and scattering; it also reduces the background of stray radiation, particularly at small scattering angles. Instrument resolution is sufficient to greatly reduce the intensity of Compton modified radiation passed by the monochromator.

2.2 Data Collection. Scattered intensities were measured with various beam divergences, ranging from 0.5° at the lowest scattering angles to 4° at the highest angles. The times for a fixed number of counts, ranging from 100,000 to 600,000, were measured at 0.25° to 1° intervals in the half-scattering angle θ. The accumulated counts were chosen to hold statistical errors in the kernel of the Fourier integral of Eq. 2.4.4 approximately uniform. The observable range of the diffractometer[21] is $0.5 \leqslant s \leqslant 16$, the scattering variable s being defined as

$$s \equiv (4\pi/\lambda)\sin\theta, \qquad (2.2.1)$$

with λ the x-ray wavelength and 2θ the scattering angle.

As the diffraction pattern of liquid water shows interference (see Section 3) to values of $s \simeq 16$, the data are appreciably more extensive than those reported by earlier workers.[1-10,20]

The Oak Ridge x-ray data on water were collected at eight temperatures between $4^{o}C$ and $200^{o}C$. The sample pressure was atmospheric at temperatures below $100^{o}C$ and equal to the vapor pressure above this temperature.[12] Triple distilled water of normal isotopic composition was used in the experiments. Heavy water (99.25% D, 1.65% 0-18, 0.12% 0-17) was studied at one temperature ($4^{o}C$).

2.3 Corrections, Scaling, and Extrapolation. The measured intensity of scattered x-radiation has to be corrected for background radiation, absorption in the sample, polarization of the x-ray beam, multiple scattering, and Compton modified radiation. For the described diffraction geometry[21] all of these corrections are either negligibly small or can be calculated with good accuracy, except for the Compton scattering which, in the case of water, is the most important single source of uncertainty in the desired result, namely the total coherently scattered intensity. Because of its importance in the present case the Compton correction will be discussed in some detail.

The intensity of Compton modified radiation[22] as a function of the variable s (defined in Eq. 2.2.1) rises rapidly to its asymptotic value, while the intensity of coherently scattered radiation has its maximum at a value of $s \simeq 2$ (for

water) and is then rapidly decreasing (see Fig. 1). All of the previously reported diffraction data on water[1-10,15-20] were collected with instruments in which all of the Compton modified radiation reached the detector. In these cases the intensity of Compton modified radiation is equal to the intensity of coherently scattered radiation at $s \simeq 5.5$, and exceeds the coherent intensity by a factor of seven at $s \simeq 16$, thus making the measurement of reliable data at large scattering angles extremely difficult. For the described diffraction geometry the intensity of Compton modified radiation rises as predicted by theory[22] at small scattering angles. However, with increasing angle the exciting source for the Compton scattering shifts from the characteristic line passed by the monochromator into the continuum. As a result the Compton scattering decreases from a maximum at intermediate angles to a small fraction of the coherent intensity at large angles. The wavelength shift of the Compton modified radiation is,[22] for MoK_α with $\lambda = 0.7107$ Å,

$$\Delta\lambda/\lambda = 0.0342\ (1 - \cos 2\theta)\ , \qquad (2.3.1)$$

and the wavelength resolution of the described diffractometer[21] is almost entirely determined by the perfection of the monochromator crystal. It can be estimated from the measured rocking curve of the crystal (half-with at half-height $\Delta\phi$) through the Bragg equation[24] as

$$\Delta\lambda/\lambda \simeq \mathrm{ctn}\phi\Delta\phi\ , \qquad (2.3.2)$$

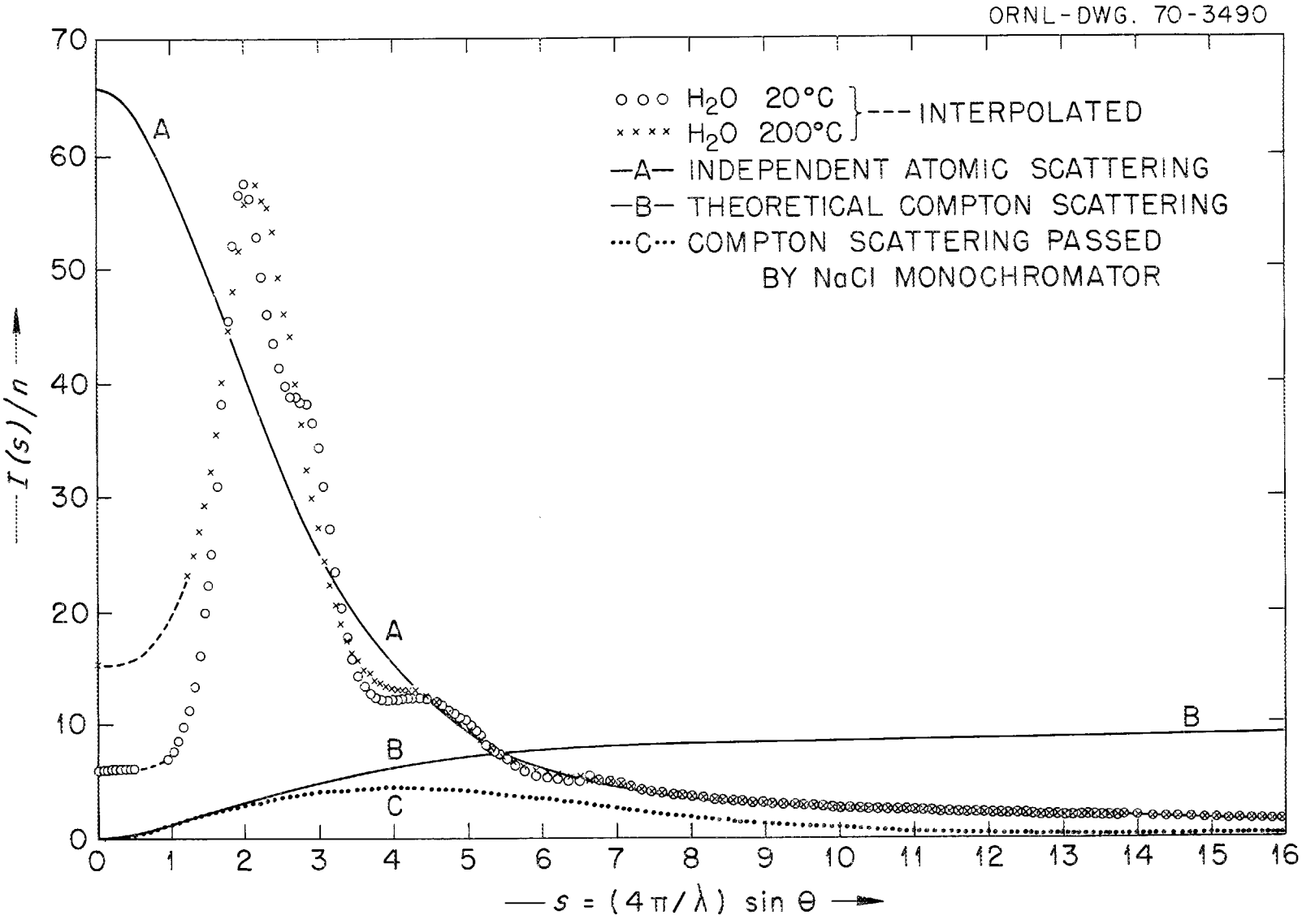


Fig. 1. Total Scattered Intensity of X-Radiation in Electron Units per Molecule for Water at Two Temperatures.

with ϕ the reflecting angle of the monochromator for radiation of wavelength λ. The water data were measured using a sodium chloride crystal set for plane (200) to reflect MoK_α radiation; for this case $\phi = 14.5^o$ and the mosaic spread of the crystal was measured as $\Delta\phi = 0.13^o$. Eq. 2.3.2 yields for the wavelength resolution a value $\Delta\lambda/\lambda \simeq 0.01$, and according to Eq. 2.3.1 the crystal monochromator should discriminate against the Compton scattering around scattering angles $2\theta \simeq 45^o$, corresponding to a value of $s \simeq 7$. Fig. 1 shows that the NaCl monochromator passes about 50% of the theoretical Compton scattering at $s \simeq 5.5$, and less than 5% at large scattering angles, qualitatively in good agreement with the above estimate.

Curve C of Fig. 1 was determined by an iterative procedure, making use of the fact that the intensity of Compton modified radiation must equal the theoretical curve B at small scattering angles, and can be determined experimentally at high angle through the use of Zr filters.[21] Once the discrimination function for a given monochromator has been determined in this way, the Compton scattering curve for any liquid can be calculated from the tabulated atomic Compton scattering amplitudes.

The absolute scale is established by normalizing the asymptote of the corrected intensity function to the theoretical independent atomic scattering (see Section 2.4) at large scattering angles. This method requires large angle data of

high precision; it is well suited to the present case because at large angles the Compton scattering is only a small fraction of the measured intensity and can be experimentally determined.[21] An alternate method[23] for the scaling of diffraction data from liquids is less suitable because it requires knowledge of the intensity function over the whole range of the scattering variable $0 \leqslant s \leqslant \infty$; in the present case scattering data are available only for the range $0.5 \leqslant s \leqslant 16$, the intensity being non-zero outside this range.

In all previously reported x-ray diffraction studies of water the intensity functions were extrapolated to zero values at zero scattering angle, a procedure which idealizes the radial distribution functions (see Section 3.1) to those for constant bulk density at large radial distances. Recently several sets of small-angle scattering data have been reported,[15-19] of which those of Hendricks[15] are the most extensive. This author found that the scattered x-ray intensity for water at nine temperatures $6.5^{o}C \leqslant t \leqslant 75^{o}C$ is constant within experimental error in the angular region $0.02 \leqslant s \leqslant 0.5$ with value I/n (see Section 2.4) equal to that calculated from bulk thermodynamic properties (Eq. 2.4.2 and 2.4.3). The intensity functions derived from the large-angle x-ray data were therefore extrapolated from the lowest values of $s \simeq 1$ to the calculated constant values in the angular region $0 \leqslant s \leqslant .3\text{-}.5$ (see Fig. 1 and Section 5).

2.4 Data Reduction. The diffraction pattern of liquid water is usually presented as a plot of the total scattered intensity of x-radiation (in electron units per molecule) against the variable s (Fig. 1). The total intensity function rises monotonically from its predicted level (Eq. 2.4.2 and 2.4.3) at zero scattering angle through a pronounced maximum, and falls off rapidly with the theoretical independent atomic scattering curve around which it oscillates with decreasing amplitude. The intensity curves of Fig. 1 for water at widely different temperatures are not very different from each other below a value of $s \sim 8$, and apparently indistinguishable from each other and from the independent atomic scattering curve above this value; this fact may serve to illustrate two points: First, the customary way of presenting diffraction data on liquids in the form of total intensity curves (as in Fig. 1) is quite insensitive to structural detail and therefore almost pointless. Second, x-ray data of considerable precision, particularly at large scattering angles, are a necessary prerequisite for the resolution of structural differences in a liquid at different temperatures.

The "structure" of a liquid is due to positional and orientational correlation between molecules. If the molecules of the liquid contain atoms of kind α,β, the radial density of distinct pairs of atoms of type α,β separated by a distance r is represented by the function $4\pi r^2\rho_{\alpha\beta}(r)$. The functions $\rho_{\alpha\beta}$ represent the average distribution of pairs both over time and

the volume of the sample; they are related[14] to the scattered intensity by the expression

$$i(s) \equiv I(s)/n - \sum_{i=1}^{m} f_i^2(s) = \sum_{\alpha=1}^{m} \sum_{\beta=1}^{m} f_\alpha(s) f_\beta(s) \int_0^\infty 4\pi r^2 [\rho_{\alpha\beta}(r) - \rho_o] \, (\sin sr/sr) dr \qquad (2.4.1)$$

in which a structural unit containing m atoms (a molecule in the case of water) is visualized as representative of the whole sample, which contains n such units and has a bulk density ρ_o. The term $\sum_{i=1}^{m} f_i^2(s)$ is the independent atomic scattering, f being the atomic scattering amplitudes. The reduced intensity i(s) is the structurally sensitive part of I(s)/n, the measured intensity scaled to one structural unit (molecule).

For a liquid composed of one well-defined molecular species which need not be monatomic the asymptotic form of Eq. 2.4.1 for small scattering angles conforms to the equation[24]

$$I(0)/nF^2 = \langle (\nu - \langle \nu \rangle)^2 \rangle / \langle \nu \rangle \qquad (2.4.2)$$

where ν is the instantaneous and $\langle \nu \rangle$ is the average number of molecules in a volume whose dimensions are large compared to a critical distance $r = r_c$, which measures the extent of short-range order in the liquid. F is the number of electrons

per molecule, and the averages are over time and the volume of the sample. A particular application of Eq. 2.4.2 concerns random equilibrium fluctuations in the local number density in a system containing one kind of molecule, in which the average density is also the most probable one, and only small fluctuations are present. Statistical mechanical considerations[25] yield for the relative variance in particle number which appears on the right side of Eq. 2.4.2

$$\langle(\nu - \langle\nu\rangle)^2\rangle / \langle\nu\rangle = kT\rho_o\chi \qquad (2.4.3)$$

where χ is the isothermal compressibility, k is the Boltzmann constant, and T is the absolute temperature.

In the case of a heteratomic liquid such as water the atom pair density functions $\rho_{\alpha\beta}(r)$ or the pair correlation functions $g_{\alpha\beta}(r) \equiv \rho_{\alpha\beta}(r)/\rho_o$ are not obtainable individually from a single diffraction experiment. It is nevertheless useful to construct a modified correlation function by Fourier transformation, namely

$$G(r) \equiv \sum_{\alpha=1}^{m} \sum_{\beta=1}^{m} G_{\alpha\beta}(r) = 1 + (1/2\pi^2\rho_o r) \int_o^\infty si(s)M(s)\sin(sr)ds \qquad (2.4.4)$$

with

$$M(s) = \left[\sum_{\alpha=1}^{m} f_\alpha(s)\right]^{-2} \qquad (2.4.5)$$

for $s \leqslant s_{max}$, the maximum value of s accessible in scattering experiments, and M(s) = 0 otherwise. Introduction of this modification function into Eq. 2.4.4 makes the product

$f_\alpha(s)f_\beta(s)M(s)$ nearly independent of s and thus removes from the resulting correlation function the average breadth of the distribution of electron density in the atoms. The modification function M(s) may, of course, be chosen at will and expressions other than the one defined in Eq. 2.4.5 have been used in the reduction of diffraction data from liquids.[1-10,20] The function chosen in this study gives Eq. 2.4.4 a logical dependence on the composition of the liquid system, reducing it to the conventional[26] expression for monatomic systems if $f_\alpha(s)f_\beta(s)M(s) = 1$, for all α,β.

The relation between component x-ray pair correlation functions $G_{\alpha\beta}(r)$ and the true atom pair correlation functions $g_{\alpha\beta}(r)$ is one of convolution[26,27]

$$G_{\alpha\beta}(r) = (1/r)\int_{-\infty}^{+\infty} ug_{\alpha\beta}(u)T_{\alpha\beta}(u-r)du \qquad (2.4.6)$$

with u a variable of integration having the same domain as r and

$$T_{\alpha\beta}(r) = (1/\pi)\int_{0}^{\infty} f_\alpha(s)f_\beta(s)M(s)\cos(sr)ds. \qquad (2.4.7)$$

The function G(r), accessible from x-ray scattering data, is thus a kind of linear combination of true atom pair correlation functions, which are convoluted with the known functions $T_{\alpha\beta}(r)$ given by Eq. 2.4.7. The factor $T_{\alpha\beta}(r)$ may be visualized as a shape function into which a pair distribution function is transformed by the combined effects of the inherent electron distribution and treatment of the x-ray data.

2.5 Errors. Three different kinds of uncertainties may affect the results of diffraction studies: Random errors, systematic errors, and the "diffraction error" resulting from truncation of the modification function in the infinite Fourier integral of Eq. 2.4.4 at finite values of the scattering variable s; the latter error affects only the correlation functions derived from the data.

Of the random errors associated with any experiment only the statistical error arising from the use of a quantum detector[28] can be estimated. It amounts to 0.3% - 0.8% in the total intensity functions (Fig. 1) and is tabulated together with the statistical errors in the reduced intensity functions in Section 5.

Systematic errors may arise from imperfections in the diffraction geometry, from uncertainties in the tabulated absorption coefficients and scattering amplitudes used in the correction and reduction of the raw data, and from uncertainties in the scaling factor which normalizes the experimental intensity curve to absolute units. The accumulated result of these systematic errors is a low frequency term in the intensity functions of Fig. 1 and 4 which may be expected to affect the correlation functions of Figs. 5 and 6 near the origin. The magnitude of this low frequency term in the intensity functions can be estimated through Fourier transformation of the difference between the observed and calculated curves in Fig. 6 at radial distances $r < 0.5$ Å (the calculated curves in

Fig. 6 will be discussed in Section 3). The systematic error in the functions si(s)M(s), estimated in this way, amounts to less than 1% corresponding to even smaller values for the total intensity curves; this uncertainty is smaller than that expected from the estimated uncertainties in the atomic scattering amplitudes[29] used in the data reduction. The systematic error in the data set collected at 50°C is somewhat larger than the above value as might have been inferred from the shape of the peak near 1 Å in the correlation functions of Fig. 5.

The "diffraction error" in the correlation functions derived from scattering data collected over only a finite range of the variable s has been discussed in its mathematical details by Waser and Schomaker.[27] The effect on G(r) can be understood through the incorporation of the cut-off into the modification function M(s) and thus inclusion in the shape functions $T_{\alpha\beta}(r)$ defined in Eq. 2.4.7. It is informative to compare correlation functions calculated from Eq. 2.4.4 for different values of the truncation s_{max} of the modification function defined in Eq. 2.4.5. Such a comparison is made in Figs. 2 and 3, for water at two temperatures, and the two sets of curves have several obvious characteristics:

The shape of maxima around 1 Å, 2.9 Å (for both temperatures), 4.5 Å, and 7 Å (at 4°C) is qualitatively not affected by the truncation limit in the range $4 \leqslant s \leqslant 16$. However, the position, height, and width of these peaks change significantly; with decreasing value of s_{max} the maximum around 2.9 Å

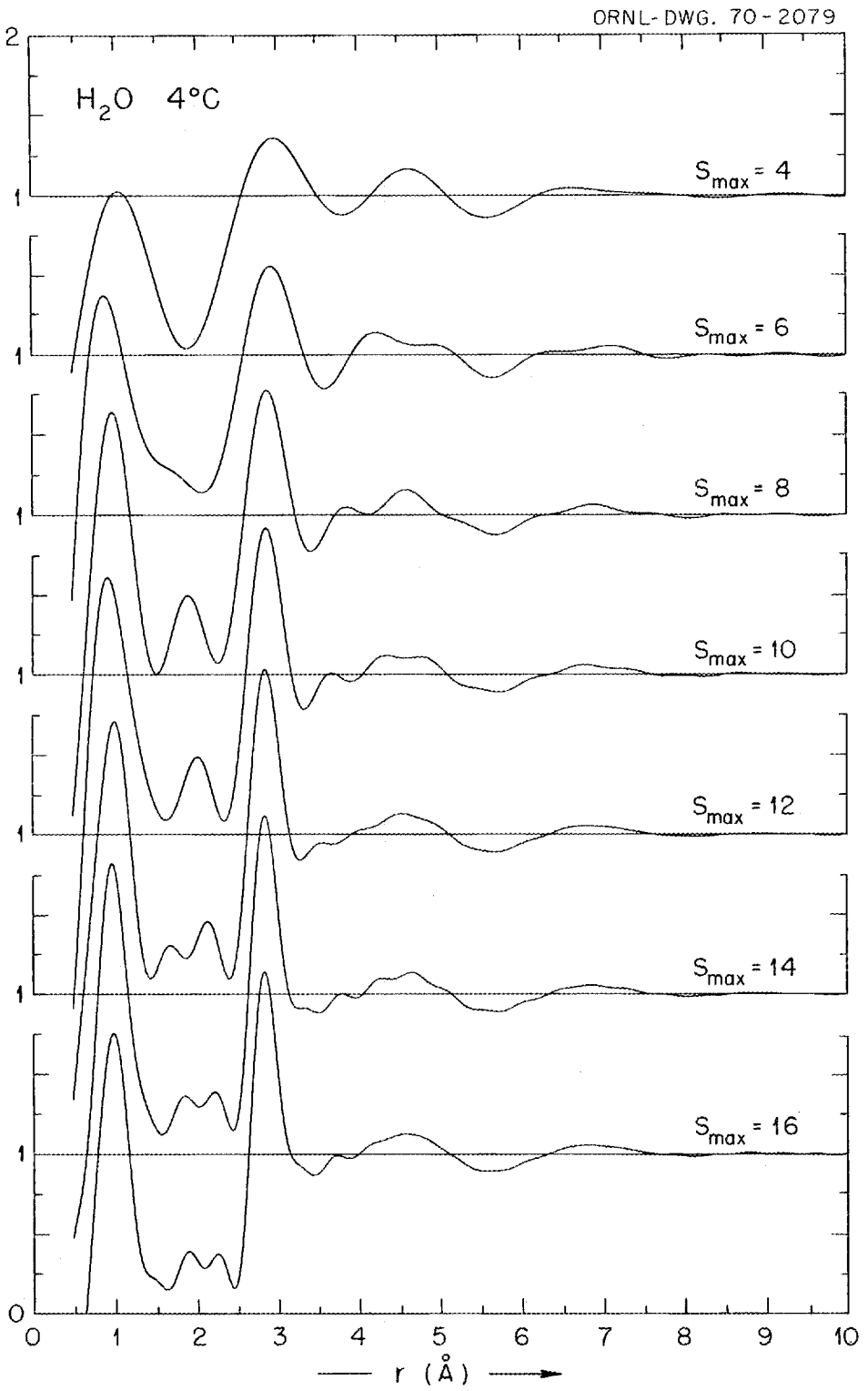


Fig. 2. X-Ray Correlation Functions G(r) for Water at 4°C for Various Values of the Truncation s_m of the Modification Function (Eq. 2.4.5) Used in the Fourier Integral of Eq. 2.4.4.

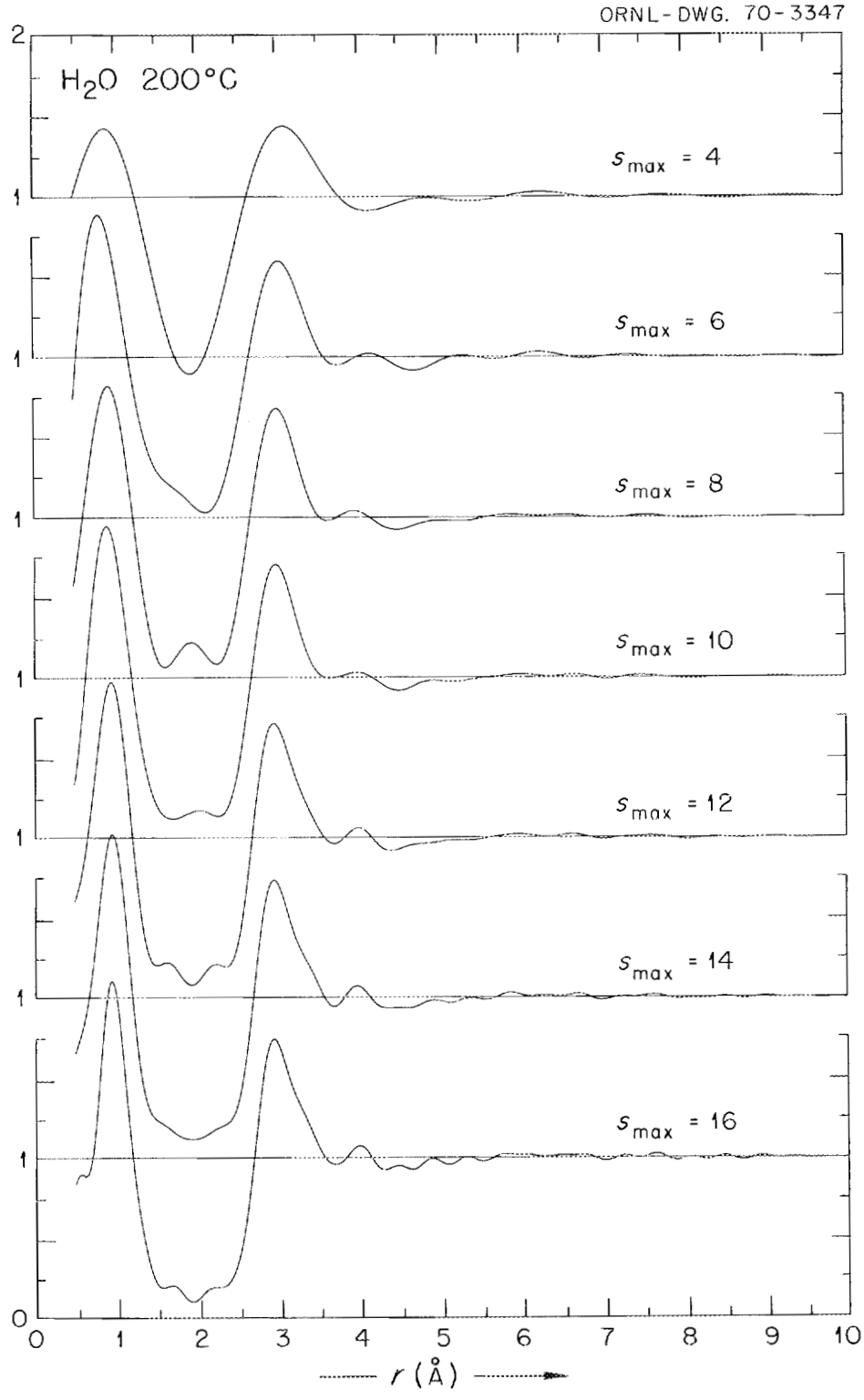


Fig. 3. X-Ray Correlation Functions G(r) for Water at 200°C for Various Values of the Truncation s_m of the Modification Function (Eq. 2.4.5) Used in the Fourier Integral of Eq. 2.4.4.

shifts towards larger distances and it broadens progressively. Apart from these major features of the correlation functions there are subsidiary features that vary even qualitatively as the truncation is changed, indicating that these features are not physically significant. The series of relatively short-wavelength ripples flanking the peak around 2.9 Å can be suppressed through the use of modification functions other than that used in the present study. However, such a procedure inevitably impairs the resolution of physically significant features in the correlation functions, particularly at small and intermediate distances.

The diffraction error in the correlation functions will always exist to some extent. However, this uncertainty need not affect the interpretation of scattering data from a liquid sample. In the following discussion all quantitative structural information on water will be derived from an analysis of the intensity functions, the correlation functions being used only to illustrate these results.

3. X-RAY DIFFRACTION PATTERN OF LIQUID WATER

The diffraction pattern of liquid water (Figs. 1 and 4) contains information about the positional correlation of oxygen and hydrogen atoms, averaged both over time and the volume of the sample. These atom pair interactions contribute to the diffraction pattern approximately as $f_\alpha f_\beta$, the product of the scattering amplitudes for atoms of kind α,β. In the

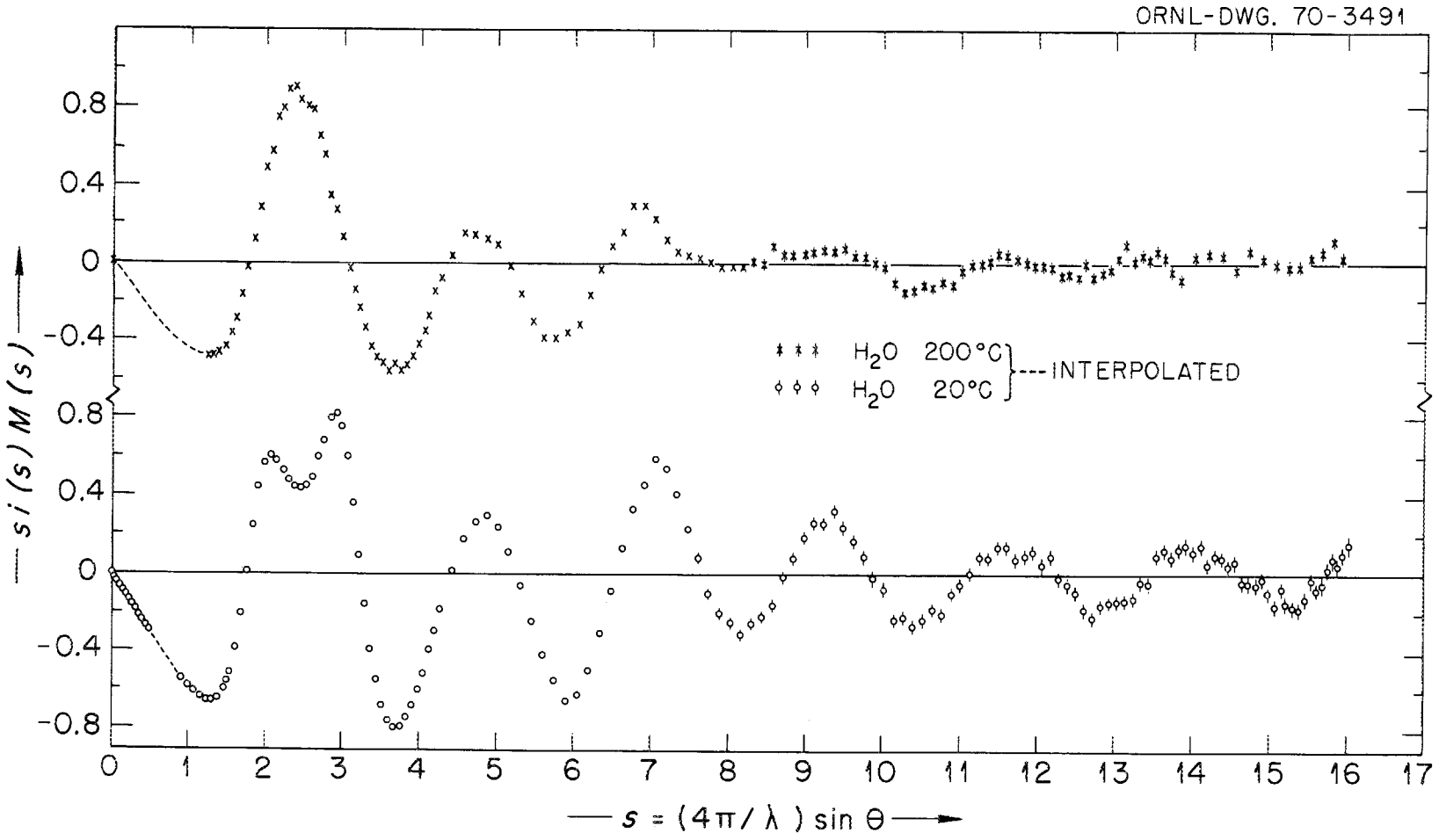


Fig. 4. Kernels of the Fourier Integral Eq. 2.4.4 for Water at Two Temperatures Represent Structurally Sensitive Part of Total Scattered Intensity Functions (Fig. 1).

case of x-rays, the scattering is predominantly due to oxygen atom pairs, but the contribution from O···H interactions is ~12% and hence not negligible; the scattering due to H···H atom pairs is only ~2% compared to O···O interactions. In contrast, in D_2O the neutron scattering amplitudes for oxygen and deuterium atoms are of nearly equal magnitude, and one would expect the neutron diffraction pattern of water to be quite different from that obtained with x-rays.[30]

The comparison of Fig. 1 with Fig. 4 further illustrates the insensitivity to structural detail, particularly at large scattering angles, of the total intensity functions in Fig. 1. In the curves of Fig. 4 the structural differences between water at 4°C and 200°C are evident. It can also be seen from Fig. 4 that the functions si(s)M(s) are oscillating around zero to values of $s \simeq 16$ and beyond; this means that the diffraction pattern of liquid water shows interference throughout this large range of scattering angles.

Throughout the following discussion, it should be borne in mind that the average spacial arrangement of atoms and molecules cannot be derived uniquely from the one-dimensional diffraction data of a liquid. It is necessary to make assumptions about the short-range order in liquid water and test the validity of these models by comparison with the x-ray data.

3.1 Radial Distribution and Short-Range Order. The x-ray atom pair correlation functions G(r) for liquid water between 4°C and 200°C, shown in Fig. 5, are significantly different

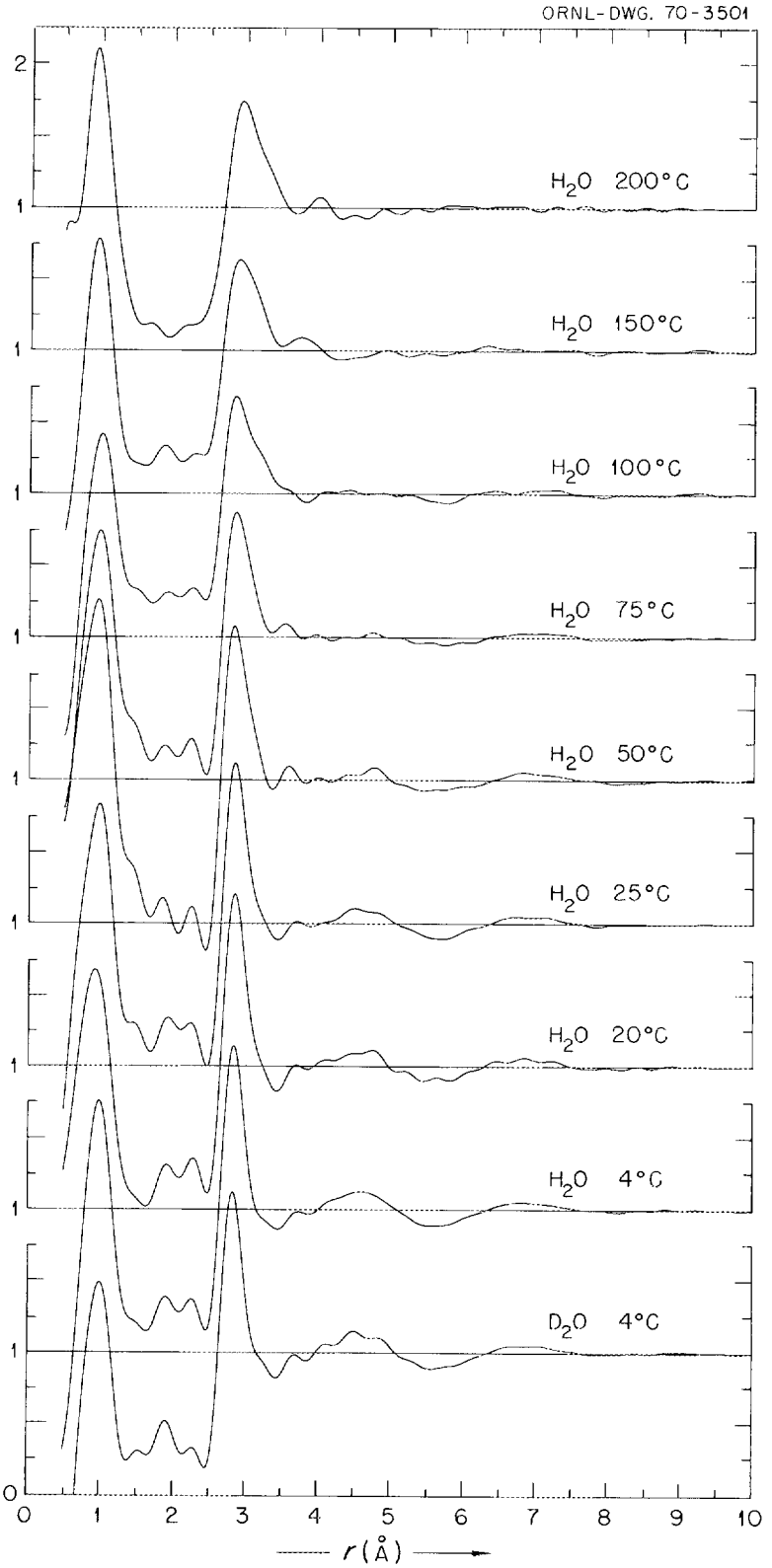


Fig. 5. X-Ray Correlation Functions G(r) for Liquid Water Represent Superpositions of Modified Atom Pair Correlation Functions g(r) Describing O-O, O-H, and H-H Interactions.

from those previously published[11-14] only in the region of radial distances $r < 2.5$ Å. The earlier curves were derived from intensity functions subjected to a correction procedure which resulted in the loss of all structural information at these small distances; no such empirical correction was used in the curves shown in Fig. 5.

The large maximum at ~1 Å must be ascribed to the intramolecular O-H interaction. Since the structure of an isolated water molecule is known from spectroscopic[31] and gas diffraction[32] studies, this part of the correlation functions can be calculated, and comparison with the curves derived from scattering data on the liquid yields a valuable criterion for their accuracy. This comparison is shown in Fig. 6 for two temperatures, and the agreement is very gratifying. The disagreement between the calculated and observed curves below 0.5 Å is the result of accumulated systematic errors in the intensity functions, as discussed in Section 2.5. The calculated curves for distances above ~1.5 Å will be discussed in Section 3.3.

The maximum at ~2.9 Å in the functions G(r) of Fig. 5 must be ascribed to interactions between oxygen atoms from neighboring water molecules. This near-neighbor distance increases from 2.84 Å at 4°C to 2.94 Å at 200°C. The values reported by Morgan and Warren[5] are larger, and this is primarily because of the lower value of s_{max}~10 (see Section 2.5). Two broad maxima around 4.5 Å and 7 Å in Fig. 5

correspond to second and higher neighbor interactions. The gradual disappearance of these features with increasing temperature indicates a decrease of the critical distance r_c which measures the extent of short-range order from about 8 Å near the melting point to about 6 Å at 200°C.

While there is no reasonable doubt about the preceding interpretation of the radial distribution curves in Fig. 5, quantitative interpretation of the curves for distances $r > 1.5$ Å is quite uncertain without additional assumptions. The calculation of average coordination numbers, in particular, is never unambiguous.[33] In this case, the lower bound of the maximum at ~2.9 Å is fairly well resolved, but the upper bound is not. Interactions with second and higher neighbors contribute significantly to the area under this peak, and proper resolution into individual components is quite uncertain even at low temperatures, where this maximum is relatively sharp. Morgan and Warren[5] derived a coordination number of ~4.4 from their curves for water at room temperature by placing the mid-position at the observed maximum of the peak and drawing the long-distance side symmetrical with the short-distance side. They also showed that it is possible to interpret the peak at ~2.9 Å as due to 3 discrete interactions and a continuous uniform density starting at ~2.7 Å; this interpretation is, however, quite arbitrary. A less arbitrary way of deriving coordination numbers from diffraction data is the following: Let us assume that the maximum at ~2.9 Å is

characteristic of the interaction of one oxygen atom with N oxygen atom neighbors separated by a Gaussian distribution of distances centered at r_o. The contribution of longer distances can be estimated as arising from a uniform distance distribution starting at the radius of a sphere of volume $(N + 1)/\rho_o$, ρ_o being the bulk density of liquid water. Using Eq. 5 of Ref. 14 and adjusting by least squares the distance r_o and the mean-square variations in both distances a value of $N = 4.4$ gives the best agreement with the experimental intensity functions for water at all temperatures; the distances r_o determined this way are listed in Table 1. But the agreement

Table 1

Average Distances r_o in Å Between Oxygen Atoms from Neighboring Water Molecules Between 4°C and 200°C. The Average Coordination Number is $N \cong 4.4$ and Independent of Temperature in this Range

°C	4	20	25	50	75	100	150	200
$r_o(H_2O)$	2.84	2.85	2.85	2.83	2.86	2.84	2.89	2.94
$r_o(D_2O)$	2.83							
Estimated Uncertainty	0.02	0.02	0.02	0.02	0.03	0.03	0.03	0.03

of this "model" (4.4 discrete O···O interactions surrounded by a uniform distance distribution) with the radial distribution

functions of water (see Fig. 1 of Ref. 14) is poor. The short-distance part of the peak at ~2.9 Å is reproduced reasonably well, but the long-distance part is not. Since, for the predominantly tetrahedral coordination indicated by this number, interactions with second neighbors would be centered at the considerably longer distance of ~4.5 Å (where a broad maximum is observed in Fig. 5), the conclusion cannot be avoided that the first coordination sphere around a water molecule is complex; the same conclusion was reached by Morgan and Warren.[5]

The only significant difference in the G(r) curves for light and heavy water at 4°C is in the region of radial distances $1.5\ \text{Å} < r < 2.5\ \text{Å}$. This region of distances is of great interest because it contains information about the relative orientation of pairs of water molecules through the O···H interaction between atoms from neighboring molecules. Unfortunately, this region is most difficult to interpret because the satellite ripples of the O···O peak around 2.9 Å (see Section 2.5 and Fig. 6) are most pronounced below 2.5 Å. It is therefore necessary to reproduce at least the major features of the G(r) curves in Fig. 5 by curves calculated for a model structure before an interpretation of this region of distances can meaningfully be attempted; this discussion is postponed until Section 3.3.

3.2 Long-Range Density Fluctuations. The fact that the correlation in Fig. 5 differ significantly from unity to radial

distances which correspond to about five molecular radii at room temperature must be ascribed to positional correlation between water molecules, that is, "structure" in liquid water. If the positional correlation were of a long-range nature (as might be the case if the molecules formed large clusters held together by hydrogen bonds, or if regions containing qualitatively different local arrangements or "phases" were present) the intensity functions shown in Fig. 1 should exhibit interference maxima and minima in the region of small scattering angles. The fact that the scattered intensity in the region $0.02 \leqslant s \leqslant 0.5$ for water below $100^{\circ}C$ is found[15] to be constant with respect to s precludes any significant variation in the pair density not included in the curves of Fig. 5. Furthermore, the value of the relative variance of the particle number derived from extrapolated small-angle scattering (Eq. 2.4.2) does not differ significantly from that predicted by Eq. 2.4.3. The random fluctuations in density expected for a liquid consisting of a single phase and a single chemical species are thus sufficient to explain the observed small-angle scattering and the small long-range variations from unity of the functions G(r) implied by it.

3.3 Models. Although a water model which scatters x-rays in exactly the same way as the real liquid cannot be proved to be unique, this agreement is necessary for the model to be tenable. A model that is to be tested against diffraction data must have a number of properties and must meet certain

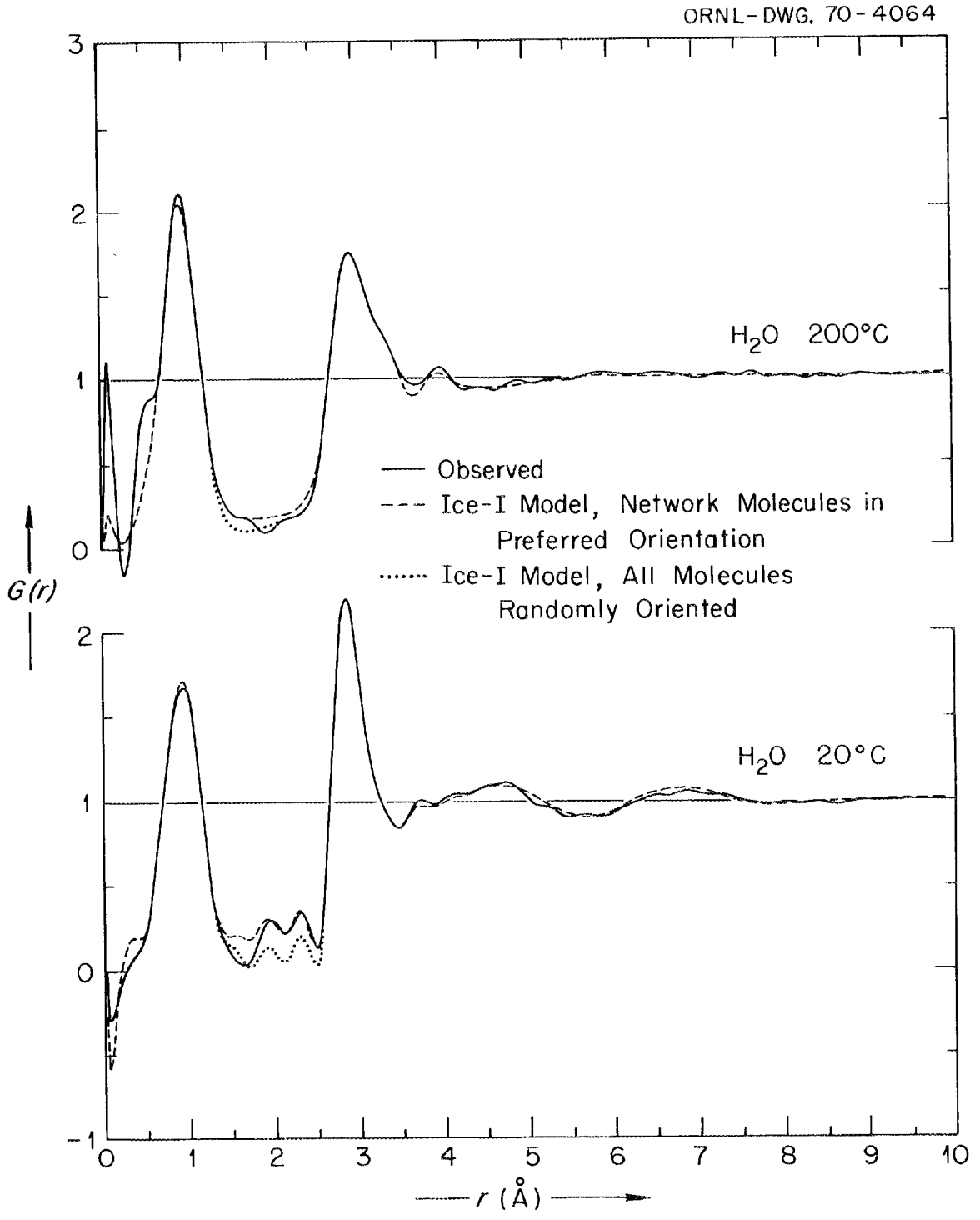


Fig. 6. Interpretation of Correlation Functions for Water at Two Temperatures. Calculated Curves for Distances r < 1.5 Å Are Model-Independent and Based on Gas Diffraction Results.

conditions[14] in order to be useful, realistic, and tractable in this context. Since most proposed models for liquid water are either incompatible with observed x-ray scattering or insufficiently defined for adequate testing,[14] only the ice-I model proposed by Samoilov[34] and specified in detail by Danford and Levy[11] will be discussed.

The ice-I model describes liquid water as an extensive three-dimensional hydrogen-bonded network, the details of which are short-lived. On the average and over short distances from any origin molecule, this network is closely related to a slightly expanded ice-I lattice. The structure of this network is very open, with spaces between groups of molecules in tetrahedral coordination sufficiently large to accommodate additional "cavity" molecules. Important characteristics of the model, descriptive of a fluid rather than a crystalline solid, are absence of long-range correlation, random occupancy of the cavities, and random network vacancies. The loss of correlation is visualized as the result of continuous small variations in instantaneous local environment. It has been embodied in the model in the form of probability distributions with mean-square variations from average separations which increase rapidly with radial distance, and the distance spectrum characteristic of the model is closely approximated by a uniform distance distribution (continuum) a few molecular radii away from any starting point.

The model is based on the following assumptions and (to keep the description as simple as possible) restrictions:

1. Each water molecule taken as the origin "sees" its neighbors in preferred average positions to radial distances of ~8 Å, with a uniform distance distribution (no structure) beyond.
2. The average arrangement of all oxygen atoms with respect to any origin is subject to the operations of the ice-I crystal space group (P6/mmc).
3. Expansion or contraction of the model network and occupancy of the cavities is permitted but constrained to conform to the experimental density. As a further constraint, deviations of the near-neighbor O···O···O angle from the tetrahedral value are not permitted, and the positions of the cavity molecules are restricted to the triad axis (Fig. 7).
4. All interactions involving hydrogen atoms are adequately described by uniform distance distributions beyond ~ 2.5 Å.

All discrete model interactions were properly weighted,[35] and the distances were related, in accordance with Assumption 2, to the nearest-neighbor distances P_1, P_2, and P_3 of Fig. 7, which were then adjusted by least-squares to seek a close fit of the model intensity functions to those derived from the diffraction data. The calculations are described in Ref. 13, where the agreement between observed and calculated intensity and radial distribution functions is shown for all temperatures

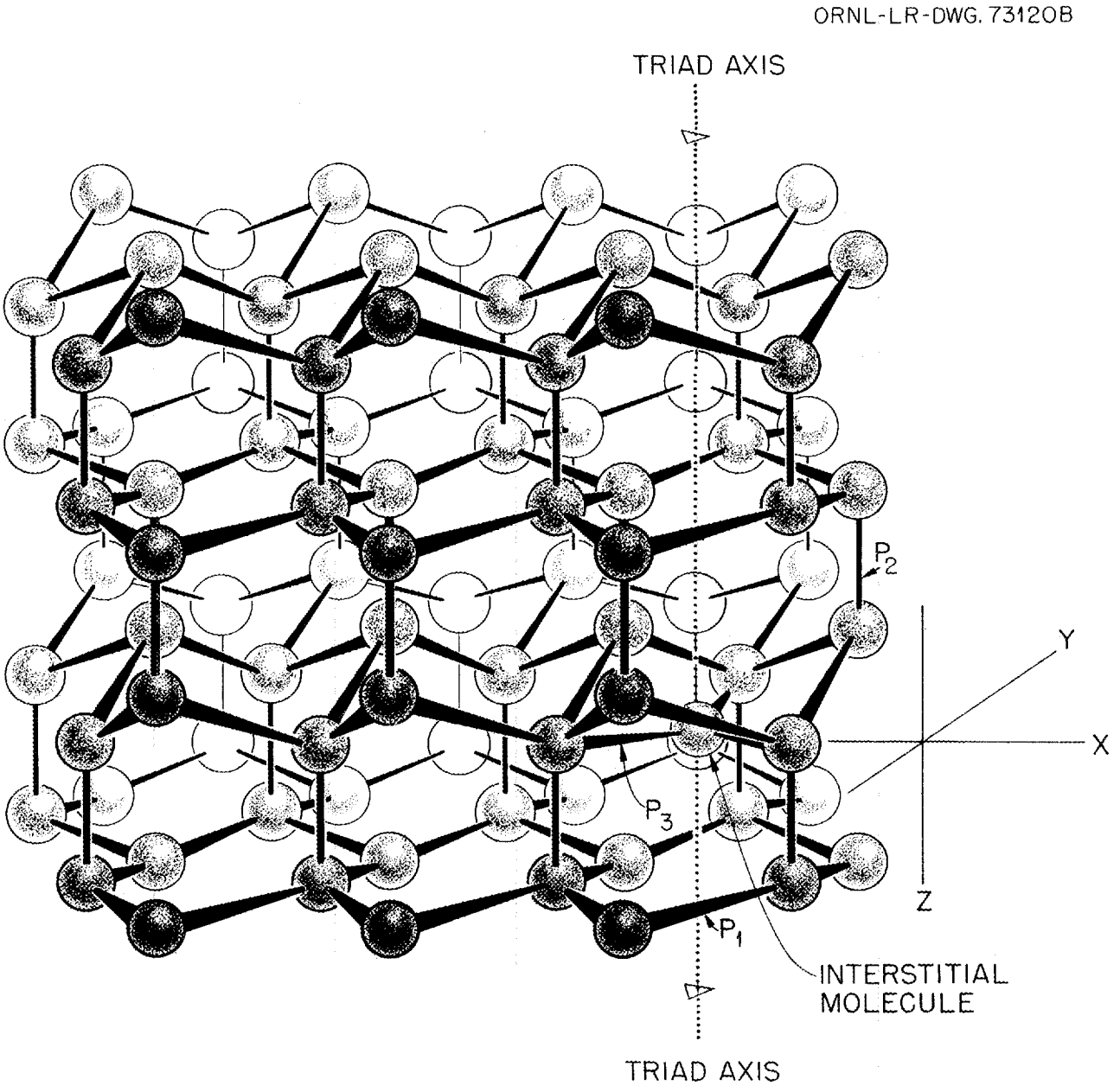


Fig. 7. Average Arrangement of Oxygen Atoms in Liquid Water (Ice-I Model) Each Network Atom Has Three Network Neighbors at a Distance P_1, and One Neighbor at a Distance P_2. Each Cavity Atom Has Three Network Neighbors at a Distance P_3, Point Symmetry D_{3h}. Large Instantaneous and Local Distortions from This Average Configuration Occur in the Liquid.

studied. Some relevant parameters of the model are presented in Section 5.2, and correlation functions calculated for the model are compared with those derived from experiment in Fig. 6 for two temperatures.

The first peak in the correlation functions of water is described by the model in terms of one network-network interaction at a distance P_2 (Fig. 7), three network-network interactions at a distance P_1, and three network-cavity interactions at a distance P_3, each of them properly weighted according to the network and cavity occupancy factors. At $4^{o}C$ the distance P_2 between network molecules related by mirror symmetry is only slightly larger than the corresponding distance in ice-I; with increasing temperature this distance (Table 2 of Section 5) contracts below the nearest-neighbor distance in ice-I. The distance P_1 between molecules related by a center of symmetry is, at $4^{o}C$, about 6% larger than the corresponding distance in ice-I, and with increasing temperature this distance goes through a maximum of 3.02 $\mathring{A}$ at $100^{o}C$. The mean-square displacements associated with these network distances show roughly the same temperature dependence. At temperatures above $100^{o}C$ the short network distance P_2 expands, and the longer P_1 distance contracts; at $200^{o}C$ the two network distances differ by an amount much smaller than their respective rms-displacements.

A molecule situated in the center of the cavity formed by adjacent layers of network molecules (Fig. 7) would have six

nearest network neighbors; the results of this study indicate that the position of the molecule is not at the cavity center but such that the angle subtended by two nearest network oxygen atoms has approximately the tetrahedral value. Thus each cavity molecule has three nearest network neighbors at a distance P_3 which is close to the longer network distance P_1.

The occupancy f_1 of network sites is 100% below 100°C; at this temperature empty network sites begin to appear. The value of f_1 drops to 87% at 150°C and 79% at 200°C. The occupancy f_2 of cavity sites increases from 45% at 4°C to 57% at 200°C. As a result, the fraction w of water molecules in network positions decreases from 82% at 4°C to 73% at 200°C. The average number of nearest-neighbor interactions calculated from these numbers is 4.4, the same results as obtained in Section 3.1 by a different method.

Since the experimental density of liquid water was used as a constraint on the occupancy of network and cavity sites, the model is in quantitative agreement with the P-V-T behavior of water over the temperature and pressure range covered by the diffraction experiments. Occupancy of cavity sites overrides network expansion up to 4°C, leading to the familiar increase in density; above 4°C network expansion at almost constant cavity occupancy results in a continuous density decrease. The model predicts three different types of hydrogen bond distributions: The bonds corresponding to the short P_2 distance must be stronger than those corresponding to

the longer P_1 network distance, and the cavity molecules may be expected to interact with the network by less directional but by no means negligible forces. It is tempting to explain the short P_2 distance in terms of relatively straight hydrogen bonds, and the longer P_1 network distance as due to slightly bent hydrogen bonds. The cavity molecules might be described as randomly oriented and, at temperatures above 100°C, also randomly located within van der Waals distance of the network molecules. This view is in agreement with the x-ray data, as illustrated in Fig. 6: Two sets of calculated curves for the distance region $1.5\ \text{Å} < r < 2.5\ \text{Å}$ are shown. Both calculated curves include the model-independent distances (0.976 Å and 1.559 Å) and variances (0.067 Å and 0.115 Å) for the intermolecular O-H and H-H interactions, taken from gas diffraction results.[32] The dotted curves incorporate all intermolecular O···H and H···H interactions as uniform distance distributions; this corresponds to random orientation of all water molecules with respect to each other. In the dashed curves of Fig. 6 it has been assumed that the network molecules are connected to their four nearest network neighbors through relatively straight hydrogen bonds, resulting in a discrete O···H distance at ~2 Å; the cavity molecules are assumed to be randomly oriented. The dashed curves, based on the latter description, agree much better with the observed ones at 20°C, but at 200°C the dotted lines for random orientation agree equally well. The rms-displacements associated with the

shortest intermolecular O···H distance are larger for H_2O than for D_2O (as might have been inferred from a comparison of the curves for $4^{o}C$ in Fig. 5) and they increase rapidly with temperature.

The complexity of the first coordination shell around a given water molecule is explained by the ice-I model in terms of distinctly different average environments of network and cavity molecules. However, both of these "species" exist in local and instantaneous configurations which are distorted from the average, and these distortions are implied by sizeable rms-variations in interatomic distance. On the scale of many molecules, the model is "single phase," homogeneous, and isotropic. There is no conflict with small-angle scattering measurements, since the superposition of interatomic distance distributions approaches a uniform distribution of distances beyond about 8 $\mathring{A}$.

4. CONCLUSIONS

The positional correlation between molecules, that is "structure" in liquid water, extends only over relatively short distances. A few molecular radii away from any starting point only the random fluctuations in density expected for a fluid consisting of a single phase and a single chemical species occur. In this respect water is no different from simple monatomic liquids.

Near the melting point the average separation between oxygen atoms from neighboring water molecules is only slightly larger than that found in ordinary ice (2.77 Å).[36] This near-neighbor distance increases gradually from 2.84 Å at 4°C to 2.94 Å at 200°C, and the corresponding maximum in the correlation functions broadens progressively with increasing temperature. The changes in position and shape of the O···O peak reflect the weakening of the O···H-O hydrogen bond at high temperatures.

The average coordination number in liquid water is independent of temperature from 4°C to 200°C and is slightly larger than four, indicating predominantly tetrahedral coordination. The distance ratio for the maxima in the correlation functions which correspond to first and second neighbor O···O interactions indicates that the average deviation from ideal tetrahedral coordination in the liquid must be quite small. On the other hand, the peak corresponding to near-neighbor O···O interactions cannot be described by a single Gaussian distance distribution, and this complexity of the first coordination shell around a given water molecule must be due to the presence in the liquid of molecules with at least two types of near-neighbor configurations. However, these "species" exist in environments which are distorted from the average so that on a scale of many molecules (sampled in small-angle scattering experiments) liquid water is "single phase," homogeneous, and isotropic.

The distribution of instantaneous and local near-neighbor O···O and O···H distances about their respective mean values is much larger in the liquid than in the solid, and hence there must also be a wide distribution of O···H-O angles about the mean value. This distribution is sharper in D_2O than in H_2O at 4^oC. The breadth of the distribution of hydrogen-bond angles increases rapidly with temperature and, at 200^oC, becomes so large that the molecules in liquid water are "seen" by x-rays as randomly oriented.

Any realistic model of water must accommodate (or at least avoid conflict with) these features which can be deduced more or less directly from the x-ray data. Of the structures which have a sufficiently detailed basis to permit calculation of radial distribution functions, only the ice-I model has been shown to give agreement with data from both large and small-angle x-ray scattering. For the few other models for which radial distribution functions have been calculated, the apparent agreement with the experimental curves for liquid water is meaningless because the computed curves do not correctly describe radial distribution in these cases.

5. APPENDIX

In Section 5.1 intensity and correlation functions for liquid water are tabulated in the format of the computer programs used. The atomic scattering amplitudes used in the data reduction are based on numerical Hartree-Fock wave functions.[29]

Values for the density and compressibility of water were also taken from the literature.[37]

In Section 5.2 some relevant parameters for the ice-I model of liquid water are tabulated.

5.1 List of Intensity and Correlation Functions. The output of the program is divided into two parts. The first presents intensity functions under the heading INTENSITIES IN ELECTRON UNITS. The second part, called RADIAL DISTRIBUTION FUNCTIONS TO 10 A, lists the correlation functions. The various terms appearing in the captions are defined as follows:

INTENSITIES IN ELECTRON UNITS

S — is the scattering variable defined in Eq. 2.2.1.

F(S) — is the theoretical independent atomic scattering per water molecule, defined in Section 2.4.

M(S) — is the modification function defined in Eq. 2.4.5.

J(S) — is the total coherently scattered intensity in electron units per water molecule, designated as I(s)/n in the previous sections.

I(S) — is the reduced intensity i(s) defined in Eq. 2.4.1, multiplied by the modification function M(s) defined in Eq. 2.4.5, designated as i(s)M(s) in the previous sections.

S*I(S) — is the kernel of the Fourier integral in Eq. 2.4.4, designated as si(s)M(s) in the previous sections.

ERROR — is the statistical error associated with the quantity in the preceding column.

RADIAL DISTRIBUTION FUNCTIONS TO 10 A

R is the radial distance in Angstrom.

G(r) is the correlation function defined in Eq. 2.4.4, obtained by numerical evaluation of the Fourier integral using the trapezoidal method.

INTENSITIES IN ELECTRON UNITS D_2O 4°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
0.0	0.660E 02	0.100E-01	0.632E 01	0.600E-01	-0.597E 00	0.0	0.0
0.100	0.659E 02	0.100E-01	0.632E 01	0.600E-01	-0.597E 00	-0.597E-01	0.601E-04
0.200	0.656E 02	0.101E-01	0.632E 01	0.600E-01	-0.597E 00	-0.119E 00	0.121E-03
0.300	0.652E 02	0.101E-01	0.632E 01	0.600E-01	-0.597E 00	-0.179E 00	0.183E-03
0.400	0.646E 02	0.102E-01	0.632E 01	0.600E-01	-0.597E 00	-0.239E 00	0.246E-03
0.500	0.638E 02	0.104E-01	0.632E 01	0.600E-01	-0.597E 00	-0.298E 00	0.311E-03
0.533	0.636E 02	0.104E-01	0.636E 01	0.598E-01	-0.596E 00	-0.318E 00	0.333E-03
0.633	0.626E 02	0.106E-01	0.654E 01	0.599E-01	-0.594E 00	-0.376E 00	0.395E-03
0.733	0.616E 02	0.108E-01	0.688E 01	0.572E-01	-0.590E 00	-0.433E 00	0.453E-03
0.833	0.603E 02	0.110E-01	0.735E 01	0.548E-01	-0.585E 00	-0.487E 00	0.504E-03
0.933	0.589E 02	0.113E-01	0.797E 01	0.517E-01	-0.577E 00	-0.539E 00	0.547E-03
1.033	0.575E 02	0.116E-01	0.872E 01	0.479E-01	-0.567E 00	-0.586E 00	0.576E-03
1.133	0.560E 02	0.120E-01	0.963E 01	0.434E-01	-0.555E 00	-0.629E 00	0.589E-03
1.233	0.544E 02	0.124E-01	0.107E 02	0.381E-01	-0.540E 00	-0.667E 00	0.581E-03
1.310	0.531E 02	0.127E-01	0.130E 02	0.457E-01	-0.509E 00	-0.667E 00	0.759E-03
1.387	0.518E 02	0.130E-01	0.160E 02	0.554E-01	-0.467E 00	-0.648E 00	0.100E-02
1.464	0.504E 02	0.134E-01	0.199E 02	0.682E-01	-0.410E 00	-0.600E 00	0.134E-02
1.541	0.491E 02	0.138E-01	0.252E 02	0.852E-01	-0.330E 00	-0.508E 00	0.182E-02
1.618	0.477E 02	0.143E-01	0.314E 02	0.105E 00	-0.232E 00	-0.376E 00	0.243E-02
1.695	0.464E 02	0.147E-01	0.386E 02	0.128E 00	-0.115E 00	-0.194E 00	0.319E-02
1.771	0.452E 02	0.152E-01	0.452E 02	0.149E 00	0.360E-02	0.638E-02	0.402E-02
1.848	0.436E 02	0.157E-01	0.500E 02	0.164E 00	0.101E 00	0.186E 00	0.478E-02
1.925	0.422E 02	0.163E-01	0.517E 02	0.170E 00	0.155E 00	0.299E 00	0.534E-02
2.002	0.408E 02	0.169E-01	0.509E 02	0.168E 00	0.171E 00	0.343E 00	0.568E-02
2.078	0.395E 02	0.175E-01	0.481E 02	0.159E 00	0.150E 00	0.312E 00	0.579E-02
2.155	0.382E 02	0.182E-01	0.448E 02	0.149E 00	0.120E 00	0.259E 00	0.583E-02
2.231	0.369E 02	0.189E-01	0.411E 02	0.137E 00	0.790E-01	0.176E 00	0.578E-02
2.308	0.356E 02	0.196E-01	0.382E 02	0.128E 00	0.515E-01	0.119E 00	0.581E-02
2.384	0.343E 02	0.204E-01	0.360E 02	0.121E 00	0.344E-01	0.820E-01	0.592E-02
2.461	0.331E 02	0.213E-01	0.348E 02	0.118E 00	0.358E-01	0.881E-01	0.616E-02
2.537	0.319E 02	0.222E-01	0.342E 02	0.116E 00	0.512E-01	0.130E 00	0.652E-02
2.614	0.307E 02	0.231E-01	0.339E 02	0.115E 00	0.727E-01	0.190E 00	0.694E-02
2.690	0.296E 02	0.241E-01	0.343E 02	0.116E 00	0.113E 00	0.304E 00	0.754E-02
2.766	0.285E 02	0.251E-01	0.346E 02	0.118E 00	0.154E 00	0.426E 00	0.817E-02
2.842	0.274E 02	0.261E-01	0.351E 02	0.120E 00	0.202E 00	0.573E 00	0.888E-02
2.918	0.264E 02	0.273E-01	0.346E 02	0.118E 00	0.223E 00	0.650E 00	0.938E-02
2.994	0.254E 02	0.284E-01	0.328E 02	0.112E 00	0.211E 00	0.631E 00	0.957E-02
3.070	0.244E 02	0.297E-01	0.296E 02	0.102E 00	0.152E 00	0.467E 00	0.932E-02
3.146	0.235E 02	0.310E-01	0.260E 02	0.912E-01	0.785E-01	0.247E 00	0.889E-02
3.222	0.226E 02	0.323E-01	0.225E 02	0.801E-01	-0.346E-02	-0.111E-01	0.835E-02
3.298	0.217E 02	0.338E-01	0.191E 02	0.695E-01	-0.892E-01	-0.294E 00	0.774E-02
3.374	0.209E 02	0.353E-01	0.167E 02	0.621E-01	-0.147E 00	-0.495E 00	0.740E-02
3.450	0.200E 02	0.369E-01	0.148E 02	0.564E-01	-0.192E 00	-0.662E 00	0.717E-02
3.525	0.193E 02	0.385E-01	0.136E 02	0.525E-01	-0.220E 00	-0.774E 00	0.712E-02
3.601	0.185E 02	0.402E-01	0.128E 02	0.501E-01	-0.230E 00	-0.830E 00	0.725E-02
3.676	0.178E 02	0.420E-01	0.122E 02	0.486E-01	-0.233E 00	-0.857E 00	0.751E-02
3.752	0.171E 02	0.439E-01	0.119E 02	0.475E-01	-0.229E 00	-0.859E 00	0.781E-02
3.827	0.164E 02	0.458E-01	0.118E 02	0.471E-01	-0.213E 00	-0.816E 00	0.826E-02
3.902	0.158E 02	0.478E-01	0.118E 02	0.475E-01	-0.191E 00	-0.745E 00	0.886E-02
3.978	0.152E 02	0.499E-01	0.118E 02	0.477E-01	-0.167E 00	-0.665E 00	0.945E-02
4.053	0.146E 02	0.520E-01	0.119E 02	0.479E-01	-0.143E 00	-0.578E 00	0.101E-01
4.128	0.141E 02	0.543E-01	0.120E 02	0.483E-01	-0.114E 00	-0.472E 00	0.108E-01
4.203	0.135E 02	0.566E-01	0.122E 02	0.491E-01	-0.766E-01	-0.322E 00	0.117E-01
4.278	0.130E 02	0.591E-01	0.120E 02	0.280E-01	-0.615E-01	-0.263E 00	0.708E-02
4.427	0.121E 02	0.641E-01	0.119E 02	0.280E-01	-0.137E-01	-0.605E-01	0.793E-02
4.576	0.113E 02	0.694E-01	0.115E 02	0.274E-01	0.188E-01	0.862E-01	0.871E-02
4.725	0.105E 02	0.753E-01	0.111E 02	0.266E-01	0.444E-01	0.210E 00	0.947E-02
4.874	0.975E 01	0.814E-01	0.104E 02	0.255E-01	0.518E-01	0.252E 00	0.101E-01
5.022	0.911E 01	0.877E-01	0.955E 01	0.240E-01	0.386E-01	0.194E 00	0.106E-01
5.170	0.851E 01	0.946E-01	0.876E 01	0.227E-01	0.239E-01	0.123E 00	0.111E-01
5.317	0.797E 01	0.102E 00	0.794E 01	0.212E-01	-0.340E-02	-0.181E-01	0.115E-01
5.464	0.750E 01	0.109E 00	0.715E 01	0.199E-01	-0.375E-01	-0.205E 00	0.118E-01
5.610	0.705E 01	0.117E 00	0.653E 01	0.188E-01	-0.617E-01	-0.346E 00	0.123E-01
5.757	0.665E 01	0.125E 00	0.594E 01	0.177E-01	-0.878E-01	-0.506E 00	0.127E-01
5.902	0.628E 01	0.133E 00	0.549E 01	0.170E-01	-0.105E 00	-0.622E 00	0.133E-01
6.047	0.595E 01	0.141E 00	0.525E 01	0.165E-01	-0.996E-01	-0.602E 00	0.141E-01
6.192	0.564E 01	0.150E 00	0.510E 01	0.161E-01	-0.810E-01	-0.502E 00	0.150E-01
6.337	0.536E 01	0.158E 00	0.497E 01	0.158E-01	-0.614E-01	-0.389E 00	0.159E-01
6.480	0.511E 01	0.167E 00	0.496E 01	0.157E-01	-0.256E-01	-0.166E 00	0.170E-01
6.624	0.488E 01	0.176E 00	0.491E 01	0.154E-01	0.656E-02	0.435E-01	0.180E-01
6.766	0.466E 01	0.185E 00	0.484E 01	0.151E-01	0.323E-01	0.219E 00	0.189E-01
6.909	0.447E 01	0.194E 00	0.477E 01	0.148E-01	0.577E-01	0.399E 00	0.198E-01

D_2O 4°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
7.051	0.430E 01	0.203E 00	0.465E 01	0.143E-01	0.712E-01	0.502E 00	0.206E-01
7.192	0.413E 01	0.213E 00	0.448E 01	0.139E-01	0.750E-01	0.540E 00	0.212E-01
7.332	0.398E 01	0.222E 00	0.426E 01	0.132E-01	0.612E-01	0.449E 00	0.215E-01
7.473	0.384E 01	0.231E 00	0.405E 01	0.127E-01	0.475E-01	0.355E 00	0.219E-01
7.612	0.372E 01	0.240E 00	0.385E 01	0.121E-01	0.312E-01	0.237E 00	0.221E-01
7.751	0.360E 01	0.249E 00	0.365E 01	0.115E-01	0.126E-01	0.977E-01	0.221E-01
7.890	0.349E 01	0.258E 00	0.346E 01	0.109E-01	-0.630E-02	-0.497E-01	0.222E-01
8.027	0.339E 01	0.266E 00	0.331E 01	0.104E-01	-0.215E-01	-0.173E 00	0.222E-01
8.164	0.329E 01	0.275E 00	0.320E 01	0.994E-02	-0.268E-01	-0.219E 00	0.223E-01
8.301	0.321E 01	0.284E 00	0.309E 01	0.951E-02	-0.339E-01	-0.281E 00	0.224E-01
8.437	0.313E 01	0.292E 00	0.303E 01	0.917E-02	-0.281E-01	-0.237E 00	0.226E-01
8.572	0.305E 01	0.300E 00	0.299E 01	0.889E-02	-0.186E-01	-0.160E 00	0.229E-01
8.707	0.298E 01	0.309E 00	0.296E 01	0.865E-02	-0.601E-02	-0.523E-01	0.232E-01
8.841	0.291E 01	0.317E 00	0.292E 01	0.840E-02	0.104E-02	0.920E-02	0.235E-01
8.974	0.285E 01	0.324E 00	0.290E 01	0.818E-02	0.153E-01	0.137E 00	0.238E-01
9.107	0.279E 01	0.332E 00	0.286E 01	0.798E-02	0.222E-01	0.202E 00	0.241E-01
9.239	0.274E 01	0.340E 00	0.281E 01	0.596E-02	0.257E-01	0.238E 00	0.187E-01
9.370	0.269E 01	0.347E 00	0.277E 01	0.578E-02	0.297E-01	0.279E 00	0.188E-01
9.500	0.264E 01	0.355E 00	0.272E 01	0.557E-02	0.284E-01	0.270E 00	0.188E-01
9.630	0.259E 01	0.362E 00	0.264E 01	0.536E-02	0.174E-01	0.168E 00	0.187E-01
9.759	0.255E 01	0.369E 00	0.258E 01	0.517E-02	0.124E-01	0.121E 00	0.186E-01
9.887	0.251E 01	0.376E 00	0.252E 01	0.498E-02	0.604E-02	0.597E-01	0.185E-01
10.015	0.247E 01	0.382E 00	0.246E 01	0.479E-02	-0.158E-02	-0.158E-01	0.184E-01
10.142	0.243E 01	0.389E 00	0.240E 01	0.462E-02	-0.122E-01	-0.124E 00	0.182E-01
10.268	0.239E 01	0.396E 00	0.235E 01	0.447E-02	-0.158E-01	-0.163E 00	0.182E-01
10.393	0.236E 01	0.403E 00	0.230E 01	0.432E-02	-0.228E-01	-0.237E 00	0.181E-01
10.517	0.233E 01	0.409E 00	0.227E 01	0.420E-02	-0.218E-01	-0.229E 00	0.181E-01
10.641	0.229E 01	0.416E 00	0.224E 01	0.411E-02	-0.206E-01	-0.219E 00	0.182E-01
10.764	0.226E 01	0.422E 00	0.222E 01	0.403E-02	-0.184E-01	-0.198E 00	0.183E-01
10.886	0.224E 01	0.429E 00	0.221E 01	0.396E-02	-0.129E-01	-0.140E 00	0.185E-01
11.007	0.221E 01	0.435E 00	0.218E 01	0.388E-02	-0.106E-01	-0.116E 00	0.186E-01
11.127	0.218E 01	0.442E 00	0.217E 01	0.382E-02	-0.555E-02	-0.617E-01	0.188E-01
11.247	0.215E 01	0.448E 00	0.216E 01	0.377E-02	0.120E-02	0.135E-01	0.190E-01
11.366	0.213E 01	0.454E 00	0.214E 01	0.372E-02	0.523E-02	0.594E-01	0.192E-01
11.483	0.210E 01	0.460E 00	0.212E 01	0.366E-02	0.922E-02	0.106E 00	0.193E-01
11.600	0.208E 01	0.466E 00	0.210E 01	0.361E-02	0.116E-01	0.135E 00	0.195E-01
11.716	0.206E 01	0.472E 00	0.208E 01	0.355E-02	0.117E-01	0.137E 00	0.196E-01
11.831	0.203E 01	0.477E 00	0.205E 01	0.349E-02	0.104E-01	0.123E 00	0.197E-01
11.946	0.201E 01	0.483E 00	0.203E 01	0.344E-02	0.105E-01	0.125E 00	0.198E-01
12.059	0.199E 01	0.488E 00	0.200E 01	0.337E-02	0.663E-02	0.799E-01	0.199E-01
12.171	0.197E 01	0.494E 00	0.197E 01	0.331E-02	0.164E-02	0.199E-01	0.199E-01
12.283	0.195E 01	0.499E 00	0.195E 01	0.326E-02	-0.947E-03	-0.116E-01	0.200E-01
12.393	0.193E 01	0.505E 00	0.192E 01	0.320E-02	-0.545E-02	-0.675E-01	0.201E-01
12.503	0.191E 01	0.510E 00	0.190E 01	0.316E-02	-0.554E-02	-0.692E-01	0.202E-01
12.611	0.189E 01	0.516E 00	0.187E 01	0.312E-02	-0.782E-02	-0.986E-01	0.203E-01
12.719	0.187E 01	0.522E 00	0.185E 01	0.308E-02	-0.107E-01	-0.136E 00	0.204E-01
12.826	0.185E 01	0.528E 00	0.183E 01	0.304E-02	-0.109E-01	-0.140E 00	0.206E-01
12.932	0.183E 01	0.534E 00	0.181E 01	0.301E-02	-0.100E-01	-0.129E 00	0.208E-01
13.036	0.181E 01	0.540E 00	0.179E 01	0.298E-02	-0.108E-01	-0.140E 00	0.210E-01
13.140	0.179E 01	0.546E 00	0.179E 01	0.297E-02	-0.515E-02	-0.676E-01	0.213E-01
13.243	0.178E 01	0.552E 00	0.176E 01	0.294E-02	-0.812E-02	-0.108E 00	0.215E-01
13.345	0.176E 01	0.558E 00	0.175E 01	0.292E-02	-0.457E-02	-0.610E-01	0.217E-01
13.445	0.174E 01	0.565E 00	0.174E 01	0.290E-02	-0.163E-03	-0.219E-02	0.220E-01
13.545	0.172E 01	0.571E 00	0.172E 01	0.288E-02	0.141E-02	0.191E-01	0.223E-01
13.644	0.170E 01	0.577E 00	0.171E 01	0.287E-02	0.431E-02	0.588E-01	0.226E-01
13.741	0.169E 01	0.583E 00	0.170E 01	0.285E-02	0.767E-02	0.105E 00	0.229E-01
13.838	0.167E 01	0.589E 00	0.168E 01	0.283E-02	0.618E-02	0.855E-01	0.230E-01
13.933	0.165E 01	0.595E 00	0.166E 01	0.281E-02	0.744E-02	0.104E 00	0.233E-01
14.028	0.164E 01	0.600E 00	0.165E 01	0.279E-02	0.102E-01	0.143E 00	0.235E-01
14.214	0.160E 01	0.612E 00	0.162E 01	0.276E-02	0.115E-01	0.163E 00	0.240E-01
14.395	0.158E 01	0.623E 00	0.159E 01	0.272E-02	0.770E-02	0.111E 00	0.244E-01
14.572	0.155E 01	0.634E 00	0.155E 01	0.267E-02	0.222E-02	0.324E-01	0.247E-01
14.744	0.152E 01	0.645E 00	0.152E 01	0.263E-02	-0.339E-02	-0.499E-01	0.250E-01
14.913	0.150E 01	0.656E 00	0.149E 01	0.258E-02	-0.100E-01	-0.149E 00	0.253E-01
15.076	0.148E 01	0.668E 00	0.146E 01	0.255E-02	-0.121E-01	-0.183E 00	0.256E-01
15.235	0.145E 01	0.679E 00	0.144E 01	0.252E-02	-0.848E-02	-0.129E 00	0.261E-01
15.389	0.143E 01	0.691E 00	0.142E 01	0.249E-02	-0.546E-02	-0.840E-01	0.265E-01
15.539	0.140E 01	0.702E 00	0.140E 01	0.246E-02	-0.464E-02	-0.722E-01	0.269E-01
15.684	0.138E 01	0.713E 00	0.138E 01	0.245E-02	-0.270E-02	-0.424E-01	0.273E-01
15.824	0.136E 01	0.723E 00	0.137E 01	0.244E-02	0.231E-02	0.366E-01	0.279E-01
15.959	0.135E 01	0.732E 00	0.135E 01	0.242E-02	0.354E-02	0.566E-01	0.283E-01

RADIAL DISTRIBUTION FUNCTIONS TO 10 A D_2O 4°C

R	G(R)	R	G(R)	R	G(R)	R	G(R)
0.0	0.0	2.50	0.2253	5.00	1.0483	7.50	1.0079
0.05	-3.9270	2.55	0.4036	5.05	1.0173	7.55	1.0040
0.10	-3.5142	2.60	0.7211	5.10	0.9906	7.60	0.9991
0.15	-2.9569	2.65	1.1344	5.15	0.9720	7.65	0.9936
0.20	-2.3973	2.70	1.5604	5.20	0.9610	7.70	0.9886
0.25	-1.9521	2.75	1.9046	5.25	0.9537	7.75	0.9852
0.30	-1.6738	2.80	2.0935	5.30	0.9455	7.80	0.9838
0.35	-1.5402	2.85	2.1003	5.35	0.9333	7.85	0.9842
0.40	-1.4746	2.90	1.9507	5.40	0.9177	7.90	0.9857
0.45	-1.3845	2.95	1.7087	5.45	0.9018	7.95	0.9873
0.50	-1.2014	3.00	1.4504	5.50	0.8895	8.00	0.9883
0.55	-0.9045	3.05	1.2358	5.55	0.8838	8.05	0.9887
0.60	-0.5198	3.10	1.0921	5.60	0.8846	8.10	0.9891
0.65	-0.1010	3.15	1.0128	5.65	0.8897	8.15	0.9900
0.70	0.2985	3.20	0.9709	5.70	0.8959	8.20	0.9919
0.75	0.6452	3.25	0.9380	5.75	0.9006	8.25	0.9945
0.80	0.9305	3.30	0.8989	5.80	0.9035	8.30	0.9968
0.85	1.1601	3.35	0.8567	5.85	0.9057	8.35	0.9979
0.90	1.3385	3.40	0.8264	5.90	0.9095	8.40	0.9974
0.95	1.4569	3.45	0.8226	5.95	0.9166	8.45	0.9956
1.00	1.4946	3.50	0.8493	6.00	0.9271	8.50	0.9935
1.05	1.4315	3.55	0.8966	6.05	0.9399	8.55	0.9922
1.10	1.2647	3.60	0.9453	6.10	0.9529	8.60	0.9926
1.15	1.0189	3.65	0.9769	6.15	0.9643	8.65	0.9947
1.20	0.7437	3.70	0.9831	6.20	0.9737	8.70	0.9979
1.25	0.4977	3.75	0.9689	6.25	0.9816	8.75	1.0011
1.30	0.3265	3.80	0.9493	6.30	0.9895	8.80	1.0035
1.35	0.2464	3.85	0.9404	6.35	0.9984	8.85	1.0046
1.40	0.2403	3.90	0.9513	6.40	1.0088	8.90	1.0048
1.45	0.2703	3.95	0.9800	6.45	1.0200	8.95	1.0046
1.50	0.2972	4.00	1.0152	6.50	1.0306	9.00	1.0045
1.55	0.3000	4.05	1.0437	6.55	1.0391	9.05	1.0044
1.60	0.2828	4.10	1.0571	6.60	1.0447	9.10	1.0041
1.65	0.2688	4.15	1.0563	6.65	1.0473	9.15	1.0031
1.70	0.2830	4.20	1.0501	6.70	1.0477	9.20	1.0013
1.75	0.3352	4.25	1.0497	6.75	1.0469	9.25	0.9992
1.80	0.4124	4.30	1.0626	6.80	1.0462	9.30	0.9974
1.85	0.4839	4.35	1.0882	6.85	1.0462	9.35	0.9966
1.90	0.5177	4.40	1.1184	6.90	1.0470	9.40	0.9971
1.95	0.4978	4.45	1.1423	6.95	1.0481	9.45	0.9983
2.00	0.4336	4.50	1.1516	7.00	1.0487	9.50	0.9992
2.05	0.3552	4.55	1.1452	7.05	1.0479	9.55	0.9992
2.10	0.2971	4.60	1.1286	7.10	1.0452	9.60	0.9977
2.15	0.2795	4.65	1.1110	7.15	1.0405	9.65	0.9951
2.20	0.2971	4.70	1.1002	7.20	1.0345	9.70	0.9926
2.25	0.3224	4.75	1.0985	7.25	1.0279	9.75	0.9910
2.30	0.3230	4.80	1.1021	7.30	1.0219	9.80	0.9910
2.35	0.2831	4.85	1.1036	7.35	1.0172	9.85	0.9923
2.40	0.2192	4.90	1.0960	7.40	1.0137	9.90	0.9941
2.45	0.1794	4.95	1.0767	7.45	1.0109	9.95	0.9955

INTENSITIES IN ELECTRON UNITS H_2O 4°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
0.0	0.660E 02	0.100E-01	0.634E 01	0.600E-01	-0.597E 00	0.0	0.0
0.100	0.659E 02	0.100E-01	0.634E 01	0.600E-01	-0.597E 00	-0.597E-01	0.601E-04
0.200	0.656E 02	0.101E-01	0.634E 01	0.600E-01	-0.597E 00	-0.119E 00	0.121E-03
0.300	0.652E 02	0.101E-01	0.634E 01	0.600E-01	-0.597E 00	-0.179E 00	0.183E-03
0.400	0.646E 02	0.102E-01	0.634E 01	0.600E-01	-0.596E 00	-0.239E 00	0.246E-03
0.500	0.638E 02	0.104E-01	0.634E 01	0.600E-01	-0.596E 00	-0.298E 00	0.311E-03
0.533	0.636E 02	0.104E-01	0.638E 01	0.599E-01	-0.596E 00	-0.318E 00	0.333E-03
0.633	0.626E 02	0.106E-01	0.660E 01	0.590E-01	-0.593E 00	-0.376E 00	0.396E-03
0.733	0.616E 02	0.108E-01	0.698E 01	0.576E-01	-0.589E 00	-0.432E 00	0.456E-03
0.833	0.603E 02	0.110E-01	0.753E 01	0.555E-01	-0.583E 00	-0.486E 00	0.511E-03
0.933	0.589E 02	0.113E-01	0.824E 01	0.526E-01	-0.574E 00	-0.536E 00	0.558E-03
1.033	0.575E 02	0.116E-01	0.912E 01	0.495E-01	-0.563E 00	-0.581E 00	0.596E-03
1.133	0.560E 02	0.120E-01	0.102E 02	0.456E-01	-0.549E 00	-0.622E 00	0.619E-03
1.233	0.544E 02	0.124E-01	0.114E 02	0.411E-01	-0.532E 00	-0.656E 00	0.626E-03
1.310	0.531E 02	0.127E-01	0.134E 02	0.480E-01	-0.504E 00	-0.660E 00	0.798E-03

H_2O 4°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
1.387	0.518E 02	0.130E-01	0.165E 02	0.584E-01	-0.460E 00	-0.638E 00	0.106E-02
1.464	0.504E 02	0.134E-01	0.204E 02	0.714E-01	-0.403E 00	-0.589E 00	0.140E-02
1.541	0.491E 02	0.138E-01	0.257E 02	0.883E-01	-0.324E 00	-0.499E 00	0.188E-02
1.618	0.477E 02	0.143E-01	0.320E 02	0.109E 00	-0.224E 00	-0.363E 00	0.251E-02
1.695	0.464E 02	0.147E-01	0.398E 02	0.133E 00	-0.100E 00	-0.170E 00	0.332E-02
1.771	0.450E 02	0.152E-01	0.466E 02	0.156E 00	0.246E-01	0.436E-01	0.419E-02
1.848	0.436E 02	0.157E-01	0.524E 02	0.174E 00	0.137E 00	0.254E 00	0.507E-02
1.925	0.422E 02	0.163E-01	0.548E 02	0.182E 00	0.206E 00	0.396E 00	0.572E-02
2.002	0.408E 02	0.169E-01	0.543E 02	0.181E 00	0.229E 00	0.458E 00	0.614E-02
2.078	0.395E 02	0.175E-01	0.518E 02	0.173E 00	0.215E 00	0.447E 00	0.631E-02
2.155	0.382E 02	0.182E-01	0.477E 02	0.161E 00	0.174E 00	0.374E 00	0.630E-02
2.231	0.369E 02	0.189E-01	0.437E 02	0.148E 00	0.128E 00	0.286E 00	0.624E-02
2.308	0.356E 02	0.196E-01	0.411E 02	0.140E 00	0.108E 00	0.250E 00	0.635E-02
2.384	0.343E 02	0.204E-01	0.387E 02	0.133E 00	0.888E-01	0.212E 00	0.646E-02
2.461	0.331E 02	0.213E-01	0.369E 02	0.127E 00	0.819E-01	0.202E 00	0.666E-02
2.537	0.319E 02	0.222E-01	0.360E 02	0.124E 00	0.912E-01	0.231E 00	0.699E-02
2.614	0.307E 02	0.231E-01	0.356E 02	0.123E 00	0.114E 00	0.298E 00	0.744E-02
2.690	0.296E 02	0.241E-01	0.359E 02	0.124E 00	0.151E 00	0.406E 00	0.803E-02
2.766	0.285E 02	0.251E-01	0.361E 02	0.125E 00	0.190E 00	0.527E 00	0.866E-02
2.842	0.274E 02	0.261E-01	0.360E 02	0.125E 00	0.223E 00	0.633E 00	0.926E-02
2.918	0.264E 02	0.273E-01	0.352E 02	0.122E 00	0.239E 00	0.697E 00	0.972E-02
2.994	0.254E 02	0.284E-01	0.333E 02	0.116E 00	0.225E 00	0.675E 00	0.992E-02
3.070	0.244E 02	0.297E-01	0.302E 02	0.107E 00	0.172E 00	0.529E 00	0.972E-02
3.146	0.235E 02	0.310E-01	0.264E 02	0.946E-01	0.891E-01	0.280E 00	0.922E-02
3.222	0.226E 02	0.323E-01	0.225E 02	0.824E-01	-0.231E-02	-0.745E-02	0.859E-02
3.298	0.217E 02	0.338E-01	0.192E 02	0.720E-01	-0.845E-01	-0.279E 00	0.803E-02
3.374	0.209E 02	0.353E-01	0.167E 02	0.643E-01	-0.145E 00	-0.491E 00	0.765E-02
3.450	0.200E 02	0.369E-01	0.149E 02	0.586E-01	-0.189E 00	-0.651E 00	0.745E-02
3.525	0.193E 02	0.385E-01	0.137E 02	0.547E-01	-0.215E 00	-0.758E 00	0.742E-02
3.601	0.185E 02	0.402E-01	0.128E 02	0.520E-01	-0.229E 00	-0.826E 00	0.753E-02
3.676	0.178E 02	0.420E-01	0.121E 02	0.502E-01	-0.238E 00	-0.875E 00	0.775E-02
3.752	0.171E 02	0.439E-01	0.118E 02	0.490E-01	-0.232E 00	-0.870E 00	0.806E-02
3.827	0.164E 02	0.458E-01	0.118E 02	0.488E-01	-0.213E 00	-0.817E 00	0.856E-02
3.902	0.158E 02	0.478E-01	0.116E 02	0.484E-01	-0.200E 00	-0.781E 00	0.903E-02
3.978	0.152E 02	0.499E-01	0.118E 02	0.487E-01	-0.172E 00	-0.685E 00	0.966E-02
4.128	0.141E 02	0.543E-01	0.119E 02	0.285E-01	-0.119E 00	-0.489E 00	0.639E-02
4.278	0.130E 02	0.591E-01	0.120E 02	0.287E-01	-0.635E-01	-0.271E 00	0.725E-02
4.427	0.121E 02	0.641E-01	0.118E 02	0.284E-01	-0.207E-01	-0.917E-01	0.807E-02
4.576	0.113E 02	0.694E-01	0.116E 02	0.281E-01	0.210E-01	0.961E-01	0.892E-02
4.725	0.105E 02	0.753E-01	0.109E 02	0.269E-01	0.319E-01	0.151E 00	0.956E-02
4.874	0.975E 01	0.814E-01	0.102E 02	0.256E-01	0.361E-01	0.176E 00	0.102E-01
5.022	0.911E 01	0.877E-01	0.956E 01	0.245E-01	0.401E-01	0.201E 00	0.108E-01
5.170	0.851E 01	0.946E-01	0.869E 01	0.229E-01	0.176E-01	0.910E-01	0.112E-01
5.317	0.797E 01	0.102E 00	0.789E 01	0.215E-01	-0.844E-02	-0.449E-01	0.116E-01
5.464	0.750E 01	0.109E 00	0.710E 01	0.201E-01	-0.437E-01	-0.239E 00	0.119E-01
5.610	0.705E 01	0.117E 00	0.648E 01	0.189E-01	-0.669E-01	-0.375E 00	0.124E-01
5.757	0.665E 01	0.125E 00	0.594E 01	0.179E-01	-0.884E-01	-0.509E 00	0.129E-01
5.902	0.628E 01	0.133E 00	0.551E 01	0.171E-01	-0.103E 00	-0.607E 00	0.134E-01
6.047	0.595E 01	0.141E 00	0.529E 01	0.166E-01	-0.939E-01	-0.568E 00	0.142E-01
6.192	0.564E 01	0.150E 00	0.510E 01	0.161E-01	-0.813E-01	-0.503E 00	0.149E-01
6.337	0.536E 01	0.158E 00	0.507E 01	0.159E-01	-0.457E-01	-0.289E 00	0.160E-01
6.480	0.511E 01	0.167E 00	0.499E 01	0.156E-01	-0.208E-01	-0.135E 00	0.169E-01
6.624	0.488E 01	0.176E 00	0.496E 01	0.153E-01	0.140E-01	0.926E-01	0.179E-01
6.766	0.466E 01	0.185E 00	0.492E 01	0.150E-01	0.470E-01	0.318E 00	0.188E-01
6.909	0.447E 01	0.194E 00	0.481E 01	0.146E-01	0.655E-01	0.452E 00	0.196E-01
7.051	0.430E 01	0.203E 00	0.464E 01	0.141E-01	0.695E-01	0.490E 00	0.202E-01
7.192	0.413E 01	0.213E 00	0.447E 01	0.136E-01	0.709E-01	0.510E 00	0.207E-01
7.332	0.398E 01	0.222E 00	0.428E 01	0.130E-01	0.671E-01	0.492E 00	0.212E-01
7.473	0.384E 01	0.231E 00	0.405E 01	0.124E-01	0.467E-01	0.349E 00	0.214E-01
7.612	0.372E 01	0.240E 00	0.382E 01	0.117E-01	0.256E-01	0.195E 00	0.214E-01
7.751	0.360E 01	0.249E 00	0.362E 01	0.111E-01	0.651E-02	0.504E-01	0.214E-01
7.890	0.349E 01	0.258E 00	0.344E 01	0.105E-01	-0.140E-01	-0.111E 00	0.213E-01
8.027	0.339E 01	0.266E 00	0.330E 01	0.999E-02	-0.250E-01	-0.201E 00	0.214E-01
8.164	0.329E 01	0.275E 00	0.317E 01	0.955E-02	-0.354E-01	-0.289E 00	0.214E-01
8.301	0.321E 01	0.284E 00	0.308E 01	0.918E-02	-0.362E-01	-0.301E 00	0.216E-01
8.437	0.313E 01	0.292E 00	0.303E 01	0.889E-02	-0.268E-01	-0.226E 00	0.219E-01
8.572	0.305E 01	0.300E 00	0.298E 01	0.859E-02	-0.220E-01	-0.189E 00	0.221E-01
8.707	0.298E 01	0.309E 00	0.296E 01	0.838E-02	-0.625E-02	-0.545E-01	0.225E-01
8.841	0.291E 01	0.317E 00	0.294E 01	0.817E-02	0.733E-02	0.648E-01	0.229E-01
8.974	0.285E 01	0.324E 00	0.290E 01	0.792E-02	0.164E-01	0.147E 00	0.231E-01
9.107	0.279E 01	0.332E 00	0.288E 01	0.631E-02	0.274E-01	0.249E 00	0.191E-01
9.239	0.274E 01	0.340E 00	0.281E 01	0.609E-02	0.243E-01	0.224E 00	0.191E-01
9.370	0.269E 01	0.347E 00	0.278E 01	0.592E-02	0.311E-01	0.291E 00	0.193E-01
9.500	0.264E 01	0.355E 00	0.272E 01	0.571E-02	0.279E-01	0.265E 00	0.192E-01
9.630	0.259E 01	0.362E 00	0.265E 01	0.552E-02	0.211E-01	0.203E 00	0.192E-01
9.759	0.255E 01	0.369E 00	0.257E 01	0.531E-02	0.829E-02	0.809E-01	0.191E-01

H_2O 4°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
9.887	0.251E 01	0.376E 00	0.250E 01	0.511E-02	-0.232E-02	-0.229E-01	0.190E-01
10.015	0.247E 01	0.382E 00	0.246E 01	0.496E-02	-0.342E-02	-0.343E-01	0.190E-01
10.142	0.243E 01	0.389E 00	0.238E 01	0.476E-02	-0.187E-01	-0.190E 00	0.188E-01
10.268	0.239E 01	0.396E 00	0.233E 01	0.461E-02	-0.252E-01	-0.259E 00	0.187E-01
10.393	0.236E 01	0.403E 00	0.229E 01	0.448E-02	-0.277E-01	-0.288E 00	0.187E-01
10.517	0.233E 01	0.409E 00	0.227E 01	0.438E-02	-0.226E-01	-0.237E 00	0.188E-01
10.641	0.229E 01	0.416E 00	0.223E 01	0.426E-02	-0.271E-01	-0.288E 00	0.189E-01
10.764	0.226E 01	0.422E 00	0.221E 01	0.419E-02	-0.210E-01	-0.226E 00	0.190E-01
10.886	0.224E 01	0.429E 00	0.220E 01	0.411E-02	-0.163E-01	-0.177E 00	0.192E-01
11.007	0.221E 01	0.435E 00	0.219E 01	0.404E-02	-0.900E-02	-0.991E-01	0.194E-01
11.127	0.218E 01	0.442E 00	0.217E 01	0.398E-02	-0.603E-02	-0.671E-01	0.196E-01
11.247	0.215E 01	0.448E 00	0.216E 01	0.393E-02	0.117E-02	0.131E-01	0.198E-01
11.366	0.213E 01	0.454E 00	0.215E 01	0.389E-02	0.784E-02	0.891E-01	0.201E-01
11.483	0.210E 01	0.460E 00	0.213E 01	0.383E-02	0.106E-01	0.122E 00	0.202E-01
11.600	0.208E 01	0.466E 00	0.210E 01	0.377E-02	0.113E-01	0.131E 00	0.204E-01
11.716	0.206E 01	0.472E 00	0.208E 01	0.371E-02	0.105E-01	0.123E 00	0.205E-01
11.831	0.203E 01	0.477E 00	0.205E 01	0.366E-02	0.918E-02	0.109E 00	0.206E-01
11.946	0.201E 01	0.483E 00	0.203E 01	0.360E-02	0.949E-02	0.113E 00	0.208E-01
12.059	0.199E 01	0.488E 00	0.200E 01	0.354E-02	0.572E-02	0.690E-01	0.209E-01
12.171	0.197E 01	0.494E 00	0.197E 01	0.348E-02	0.115E-02	0.140E-01	0.209E-01
12.283	0.195E 01	0.499E 00	0.194E 01	0.343E-02	-0.216E-02	-0.265E-01	0.210E-01
12.393	0.193E 01	0.505E 00	0.191E 01	0.337E-02	-0.757E-02	-0.938E-01	0.211E-01
12.503	0.191E 01	0.510E 00	0.190E 01	0.333E-02	-0.730E-02	-0.912E-01	0.212E-01
12.611	0.189E 01	0.516E 00	0.187E 01	0.328E-02	-0.955E-02	-0.120E 00	0.214E-01
12.719	0.187E 01	0.522E 00	0.184E 01	0.323E-02	-0.135E-01	-0.172E 00	0.215E-01
12.826	0.185E 01	0.528E 00	0.182E 01	0.319E-02	-0.173E-01	-0.222E 00	0.216E-01
12.932	0.183E 01	0.534E 00	0.181E 01	0.317E-02	-0.115E-01	-0.149E 00	0.219E-01
13.036	0.181E 01	0.540E 00	0.179E 01	0.313E-02	-0.112E-01	-0.146E 00	0.221E-01
13.140	0.179E 01	0.546E 00	0.178E 01	0.311E-02	-0.985E-02	-0.129E 00	0.223E-01
13.243	0.178E 01	0.552E 00	0.177E 01	0.310E-02	-0.320E-02	-0.423E-01	0.227E-01
13.345	0.176E 01	0.558E 00	0.175E 01	0.306E-02	-0.570E-02	-0.761E-01	0.228E-01
13.445	0.174E 01	0.565E 00	0.174E 01	0.305E-02	-0.176E-02	-0.236E-01	0.231E-01
13.545	0.172E 01	0.571E 00	0.173E 01	0.304E-02	0.493E-02	0.668E-01	0.235E-01
13.644	0.170E 01	0.577E 00	0.172E 01	0.302E-02	0.753E-02	0.103E 00	0.238E-01
13.741	0.169E 01	0.583E 00	0.170E 01	0.301E-02	0.934E-02	0.128E 00	0.241E-01
13.838	0.167E 01	0.589E 00	0.169E 01	0.299E-02	0.110E-01	0.152E 00	0.244E-01
13.933	0.165E 01	0.595E 00	0.167E 01	0.296E-02	0.104E-01	0.145E 00	0.246E-01
14.028	0.164E 01	0.600E 00	0.165E 01	0.294E-02	0.910E-02	0.128E 00	0.248E-01
14.214	0.160E 01	0.612E 00	0.162E 01	0.274E-02	0.695E-02	0.988E-01	0.238E-01
14.305	0.158E 01	0.623E 00	0.158E 01	0.270E-02	0.480E-02	0.691E-01	0.242E-01
14.572	0.155E 01	0.634E 00	0.155E 01	0.266E-02	0.133E-02	0.194E-01	0.245E-01
14.744	0.152E 01	0.645E 00	0.152E 01	0.261E-02	-0.366E-02	-0.539E-01	0.248E-01
14.913	0.150E 01	0.656E 00	0.149E 01	0.257E-02	-0.695E-02	-0.104E 00	0.252E-01
15.076	0.148E 01	0.668E 00	0.147E 01	0.255E-02	-0.371E-02	-0.559E-01	0.257E-01
15.235	0.145E 01	0.679E 00	0.144E 01	0.252E-02	-0.751E-02	-0.114E 00	0.260E-01
15.389	0.143E 01	0.691E 00	0.142E 01	0.249E-02	-0.347E-02	-0.535E-01	0.265E-01
15.539	0.140E 01	0.702E 00	0.140E 01	0.246E-02	-0.527E-02	-0.819E-01	0.269E-01
15.684	0.138E 01	0.713E 00	0.138E 01	0.245E-02	-0.258E-03	-0.405E-02	0.274E-01
15.824	0.136E 01	0.723E 00	0.136E 01	0.243E-02	-0.454E-03	-0.718E-02	0.278E-01
15.959	0.135E 01	0.732E 00	0.135E 01	0.241E-02	0.264E-02	0.421E-01	0.282E-01

RADIAL DISTRIBUTION FUNCTIONS TO 10 A

H_2O 4°C

R	G(R)	R	G(R)	R	G(R)	R	G(R)
0.0	0.0	2.50	0.1804	5.00	1.0347	7.50	1.0084
0.05	-4.3430	2.55	0.3424	5.05	1.0174	7.55	1.0039
0.10	-3.8639	2.60	0.6483	5.10	1.0013	7.60	0.9996
0.15	-3.1920	2.65	1.0582	5.15	0.9857	7.65	0.9957
0.20	-2.4711	2.70	1.4834	5.20	0.9698	7.70	0.9928
0.25	-1.8316	2.75	1.8616	5.25	0.9529	7.75	0.9909
0.30	-1.3537	2.80	2.0872	5.30	0.9354	7.80	0.9901
0.35	-1.0521	2.85	2.1352	5.35	0.9186	7.85	0.9898
0.40	-0.8847	2.90	2.0199	5.40	0.9045	7.90	0.9893
0.45	-0.7793	2.95	1.7948	5.45	0.8945	7.95	0.9881
0.50	-0.6647	3.00	1.5312	5.50	0.8893	8.00	0.9858
0.55	-0.4935	3.05	1.2925	5.55	0.8879	8.05	0.9832
0.60	-0.2505	3.10	1.1167	5.60	0.8886	8.10	0.9813
0.65	0.0532	3.15	1.0106	5.65	0.8901	8.15	0.9809
0.70	0.3926	3.20	0.9576	5.70	0.8916	8.20	0.9826
0.75	0.7405	3.25	0.9318	5.75	0.8936	8.25	0.9859
0.80	1.0724	3.30	0.9123	5.80	0.8972	8.30	0.9897

H_2O 4°C

R	G(R)	R	G(R)	R	G(R)	R	G(R)
0.85	1.3649	3.35	0.8906	5.85	0.9036	8.35	0.9928
0.90	1.5925	3.40	0.8708	5.90	0.9130	8.40	0.9944
0.95	1.7278	3.45	0.8622	5.95	0.9247	8.45	0.9944
1.00	1.7480	3.50	0.8717	6.00	0.9372	8.50	0.9938
1.05	1.6443	3.55	0.8982	6.05	0.9489	8.55	0.9939
1.10	1.4317	3.60	0.9329	6.10	0.9587	8.60	0.9956
1.15	1.1492	3.65	0.9641	6.15	0.9669	8.65	0.9989
1.20	0.8509	3.70	0.9824	6.20	0.9743	8.70	1.0030
1.25	0.5901	3.75	0.9857	6.25	0.9820	8.75	1.0063
1.30	0.4016	3.80	0.9787	6.30	0.9908	8.80	1.0075
1.35	0.2927	3.85	0.9703	6.35	1.0007	8.85	1.0064
1.40	0.2446	3.90	0.9688	6.40	1.0110	8.90	1.0035
1.45	0.2257	3.95	0.9781	6.45	1.0209	8.95	1.0004
1.50	0.2084	4.00	0.9967	6.50	1.0294	9.00	0.9983
1.55	0.1816	4.05	1.0194	6.55	1.0364	9.05	0.9982
1.60	0.1534	4.10	1.0404	6.60	1.0418	9.10	0.9996
1.65	0.1431	4.15	1.0563	6.65	1.0461	9.15	1.0016
1.70	0.1662	4.20	1.0670	6.70	1.0494	9.20	1.0027
1.75	0.2235	4.25	1.0746	6.75	1.0516	9.25	1.0021
1.80	0.2975	4.30	1.0821	6.80	1.0527	9.30	0.9999
1.85	0.3605	4.35	1.0912	6.85	1.0524	9.35	0.9971
1.90	0.3889	4.40	1.1015	6.90	1.0509	9.40	0.9950
1.95	0.3756	4.45	1.1115	6.95	1.0487	9.45	0.9945
2.00	0.3349	4.50	1.1190	7.00	1.0460	9.50	0.9957
2.05	0.2944	4.55	1.1229	7.05	1.0434	9.55	0.9975
2.10	0.2799	4.60	1.1231	7.10	1.0409	9.60	0.9987
2.15	0.3005	4.65	1.1204	7.15	1.0383	9.65	0.9981
2.20	0.3416	4.70	1.1154	7.20	1.0352	9.70	0.9957
2.25	0.3724	4.75	1.1083	7.25	1.0315	9.75	0.9923
2.30	0.3627	4.80	1.0986	7.30	1.0272	9.80	0.9893
2.35	0.3029	4.85	1.0858	7.35	1.0226	9.85	0.9882
2.40	0.2159	4.90	1.0702	7.40	1.0178	9.90	0.9896
2.45	0.1540	4.95	1.0527	7.45	1.0130	9.95	0.9932

INTENSITIES IN ELECTRON UNITS H_2O 20°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
0.0	0.660E 02	0.100E-01	0.620E 01	0.600E-01	-0.598E 00	0.0	0.0
0.010	0.660E 02	0.100E-01	0.620E 01	0.600E-01	-0.598E 00	-0.598E-02	0.600E-05
0.020	0.660E 02	0.100E-01	0.620E 01	0.600E-01	-0.598E 00	-0.120E-01	0.120E-04
0.030	0.660E 02	0.100E-01	0.620E 01	0.600E-01	-0.598E 00	-0.179E-01	0.180E-04
0.040	0.660E 02	0.100E-01	0.620E 01	0.600E-01	-0.598E 00	-0.239E-01	0.240E-04
0.050	0.660E 02	0.100E-01	0.620E 01	0.600E-01	-0.598E 00	-0.299E-01	0.300E-04
0.060	0.659E 02	0.100E-01	0.620E 01	0.600E-01	-0.598E 00	-0.359E-01	0.360E-04
0.070	0.659E 02	0.100E-01	0.620E 01	0.600E-01	-0.598E 00	-0.419E-01	0.421E-04
0.080	0.659E 02	0.100E-01	0.620E 01	0.600E-01	-0.598E 00	-0.478E-01	0.481E-04
0.090	0.659E 02	0.100E-01	0.620E 01	0.600E-01	-0.598E 00	-0.538E-01	0.541E-04
0.100	0.659E 02	0.100E-01	0.620E 01	0.600E-01	-0.598E 00	-0.598E-01	0.601E-04
0.110	0.658E 02	0.100E-01	0.620E 01	0.600E-01	-0.598E 00	-0.658E-01	0.662E-04
0.120	0.658E 02	0.100E-01	0.620E 01	0.600E-01	-0.598E 00	-0.718E-01	0.722E-04
0.130	0.658E 02	0.100E-01	0.620E 01	0.600E-01	-0.598E 00	-0.777E-01	0.783E-04
0.140	0.658E 02	0.100E-01	0.620E 01	0.600E-01	-0.598E 00	-0.837E-01	0.843E-04
0.150	0.657E 02	0.100E-01	0.620E 01	0.600E-01	-0.598E 00	-0.897E-01	0.904E-04
0.160	0.657E 02	0.100E-01	0.620E 01	0.600E-01	-0.598E 00	-0.957E-01	0.965E-04
0.170	0.657E 02	0.101E-01	0.620E 01	0.600E-01	-0.598E 00	-0.102E 00	0.103E-03
0.180	0.657E 02	0.101E-01	0.620E 01	0.600E-01	-0.598E 00	-0.108E 00	0.109E-03
0.190	0.656E 02	0.101E-01	0.620E 01	0.600E-01	-0.598E 00	-0.114E 00	0.115E-03
0.200	0.656E 02	0.101E-01	0.620E 01	0.600E-01	-0.598E 00	-0.120E 00	0.121E-03
0.210	0.655E 02	0.101E-01	0.620E 01	0.600E-01	-0.598E 00	-0.126E 00	0.127E-03
0.220	0.655E 02	0.101E-01	0.620E 01	0.600E-01	-0.598E 00	-0.132E 00	0.133E-03
0.230	0.655E 02	0.101E-01	0.620E 01	0.600E-01	-0.598E 00	-0.138E 00	0.139E-03
0.240	0.654E 02	0.101E-01	0.620E 01	0.600E-01	-0.598E 00	-0.144E 00	0.145E-03
0.250	0.654E 02	0.101E-01	0.620E 01	0.600E-01	-0.598E 00	-0.150E 00	0.152E-03
0.260	0.653E 02	0.101E-01	0.620E 01	0.600E-01	-0.598E 00	-0.155E 00	0.158E-03
0.270	0.653E 02	0.101E-01	0.620E 01	0.600E-01	-0.598E 00	-0.161E 00	0.164E-03
0.280	0.653E 02	0.101E-01	0.620E 01	0.600E-01	-0.598E 00	-0.167E 00	0.170E-03
0.290	0.652E 02	0.101E-01	0.620E 01	0.600E-01	-0.598E 00	-0.173E 00	0.176E-03
0.300	0.652E 02	0.101E-01	0.620E 01	0.600E-01	-0.598E 00	-0.179E 00	0.183E-03
0.310	0.651E 02	0.102E-01	0.620E 01	0.600E-01	-0.598E 00	-0.185E 00	0.189E-03
0.320	0.650E 02	0.102E-01	0.620E 01	0.600E-01	-0.598E 00	-0.191E 00	0.195E-03
0.330	0.650E 02	0.102E-01	0.620E 01	0.600E-01	-0.598E 00	-0.197E 00	0.201E-03
0.340	0.649E 02	0.102E-01	0.620E 01	0.600E-01	-0.598E 00	-0.203E 00	0.208E-03
0.350	0.649E 02	0.102E-01	0.620E 01	0.600E-01	-0.598E 00	-0.209E 00	0.214E-03

H_2O 20°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
0.355	0.648E 02	0.102E-01	0.620E 01	0.600E-01	-0.598E 00	-0.213E 00	0.217E-03
0.365	0.648E 02	0.102E-01	0.620E 01	0.600E-01	-0.598E 00	-0.218E 00	0.224E-03
0.375	0.647E 02	0.102E-01	0.620E 01	0.599E-01	-0.598E 00	-0.224E 00	0.230E-03
0.385	0.647E 02	0.102E-01	0.620E 01	0.599E-01	-0.598E 00	-0.230E 00	0.236E-03
0.395	0.646E 02	0.102E-01	0.621E 01	0.599E-01	-0.598E 00	-0.236E 00	0.242E-03
0.405	0.645E 02	0.103E-01	0.621E 01	0.598E-01	-0.598E 00	-0.242E 00	0.248E-03
0.415	0.645E 02	0.103E-01	0.621E 01	0.597E-01	-0.598E 00	-0.248E 00	0.255E-03
0.425	0.644E 02	0.103E-01	0.621E 01	0.596E-01	-0.598E 00	-0.254E 00	0.261E-03
0.435	0.643E 02	0.103E-01	0.622E 01	0.595E-01	-0.598E 00	-0.260E 00	0.267E-03
0.445	0.643E 02	0.103E-01	0.622E 01	0.594E-01	-0.598E 00	-0.266E 00	0.272E-03
0.455	0.642E 02	0.103E-01	0.623E 01	0.593E-01	-0.598E 00	-0.272E 00	0.278E-03
0.465	0.641E 02	0.103E-01	0.623E 01	0.591E-01	-0.598E 00	-0.278E 00	0.284E-03
0.475	0.640E 02	0.103E-01	0.624E 01	0.590E-01	-0.598E 00	-0.284E 00	0.290E-03
0.485	0.640E 02	0.104E-01	0.624E 01	0.588E-01	-0.597E 00	-0.290E 00	0.296E-03
0.495	0.639E 02	0.104E-01	0.625E 01	0.587E-01	-0.597E 00	-0.296E 00	0.301E-03
0.505	0.638E 02	0.104E-01	0.625E 01	0.585E-01	-0.597E 00	-0.302E 00	0.307E-03
0.515	0.637E 02	0.104E-01	0.626E 01	0.583E-01	-0.597E 00	-0.308E 00	0.312E-03
0.525	0.636E 02	0.104E-01	0.627E 01	0.581E-01	-0.597E 00	-0.314E 00	0.318E-03
0.535	0.635E 02	0.104E-01	0.628E 01	0.579E-01	-0.597E 00	-0.320E 00	0.323E-03
0.545	0.635E 02	0.104E-01	0.628E 01	0.576E-01	-0.597E 00	-0.326E 00	0.328E-03
0.555	0.634E 02	0.105E-01	0.629E 01	0.574E-01	-0.597E 00	-0.331E 00	0.333E-03
0.565	0.633E 02	0.105E-01	0.630E 01	0.571E-01	-0.597E 00	-0.337E 00	0.338E-03
0.575	0.632E 02	0.105E-01	0.631E 01	0.569E-01	-0.597E 00	-0.343E 00	0.343E-03
0.585	0.631E 02	0.105E-01	0.632E 01	0.566E-01	-0.596E 00	-0.349E 00	0.348E-03
0.595	0.630E 02	0.105E-01	0.633E 01	0.563E-01	-0.596E 00	-0.355E 00	0.353E-03
0.605	0.629E 02	0.105E-01	0.634E 01	0.560E-01	-0.596E 00	-0.361E 00	0.357E-03
0.615	0.628E 02	0.106E-01	0.635E 01	0.557E-01	-0.596E 00	-0.367E 00	0.362E-03
0.625	0.627E 02	0.106E-01	0.637E 01	0.554E-01	-0.596E 00	-0.373E 00	0.366E-03
0.635	0.626E 02	0.106E-01	0.638E 01	0.550E-01	-0.596E 00	-0.379E 00	0.370E-03
0.645	0.625E 02	0.106E-01	0.639E 01	0.547E-01	-0.596E 00	-0.384E 00	0.374E-03
0.655	0.624E 02	0.106E-01	0.640E 01	0.543E-01	-0.595E 00	-0.390E 00	0.378E-03
0.665	0.623E 02	0.107E-01	0.642E 01	0.539E-01	-0.595E 00	-0.396E 00	0.382E-03
0.675	0.622E 02	0.107E-01	0.643E 01	0.535E-01	-0.595E 00	-0.402E 00	0.386E-03
0.685	0.621E 02	0.107E-01	0.644E 01	0.531E-01	-0.595E 00	-0.408E 00	0.390E-03
0.695	0.620E 02	0.107E-01	0.646E 01	0.527E-01	-0.595E 00	-0.414E 00	0.393E-03
0.705	0.619E 02	0.107E-01	0.647E 01	0.523E-01	-0.595E 00	-0.419E 00	0.396E-03
0.715	0.618E 02	0.108E-01	0.649E 01	0.519E-01	-0.594E 00	-0.425E 00	0.399E-03
0.725	0.616E 02	0.108E-01	0.650E 01	0.514E-01	-0.594E 00	-0.431E 00	0.402E-03
0.735	0.615E 02	0.108E-01	0.652E 01	0.510E-01	-0.594E 00	-0.437E 00	0.405E-03
0.745	0.614E 02	0.108E-01	0.654E 01	0.505E-01	-0.594E 00	-0.443E 00	0.408E-03
0.755	0.613E 02	0.108E-01	0.655E 01	0.500E-01	-0.594E 00	-0.448E 00	0.410E-03
0.765	0.612E 02	0.109E-01	0.657E 01	0.496E-01	-0.593E 00	-0.454E 00	0.412E-03
0.775	0.611E 02	0.109E-01	0.659E 01	0.490E-01	-0.593E 00	-0.460E 00	0.414E-03
0.785	0.609E 02	0.109E-01	0.661E 01	0.485E-01	-0.593E 00	-0.466E 00	0.416E-03
0.795	0.608E 02	0.109E-01	0.663E 01	0.480E-01	-0.593E 00	-0.471E 00	0.418E-03
0.805	0.607E 02	0.110E-01	0.664E 01	0.475E-01	-0.592E 00	-0.477E 00	0.419E-03
0.815	0.606E 02	0.110E-01	0.666E 01	0.469E-01	-0.592E 00	-0.483E 00	0.420E-03
0.825	0.604E 02	0.110E-01	0.668E 01	0.464E-01	-0.592E 00	-0.489E 00	0.421E-03
0.835	0.603E 02	0.110E-01	0.670E 01	0.458E-01	-0.592E 00	-0.494E 00	0.422E-03
0.845	0.602E 02	0.111E-01	0.672E 01	0.452E-01	-0.591E 00	-0.500E 00	0.423E-03
0.855	0.600E 02	0.111E-01	0.675E 01	0.446E-01	-0.591E 00	-0.506E 00	0.423E-03
0.865	0.599E 02	0.111E-01	0.677E 01	0.440E-01	-0.591E 00	-0.511E 00	0.423E-03
0.875	0.598E 02	0.111E-01	0.679E 01	0.434E-01	-0.591E 00	-0.517E 00	0.423E-03
0.885	0.596E 02	0.112E-01	0.681E 01	0.427E-01	-0.590E 00	-0.523E 00	0.423E-03
0.895	0.595E 02	0.112E-01	0.683E 01	0.421E-01	-0.590E 00	-0.528E 00	0.422E-03
0.905	0.593E 02	0.112E-01	0.686E 01	0.414E-01	-0.590E 00	-0.534E 00	0.421E-03
0.915	0.592E 02	0.113E-01	0.688E 01	0.408E-01	-0.589E 00	-0.539E 00	0.420E-03
0.925	0.591E 02	0.113E-01	0.691E 01	0.401E-01	-0.589E 00	-0.545E 00	0.419E-03
1.002	0.579E 02	0.115E-01	0.756E 01	0.435E-01	-0.581E 00	-0.583E 00	0.503E-03
1.079	0.568E 02	0.118E-01	0.862E 01	0.480E-01	-0.568E 00	-0.613E 00	0.611E-03
1.156	0.556E 02	0.121E-01	0.985E 01	0.529E-01	-0.552E 00	-0.638E 00	0.737E-03
1.233	0.544E 02	0.124E-01	0.114E 02	0.586E-01	-0.532E 00	-0.656E 00	0.893E-03
1.310	0.531E 02	0.127E-01	0.135E 02	0.653E-01	-0.503E 00	-0.659E 00	0.108E-02
1.387	0.518E 02	0.130E-01	0.163E 02	0.732E-01	-0.462E 00	-0.641E 00	0.132E-02
1.464	0.504E 02	0.134E-01	0.202E 02	0.829E-01	-0.406E 00	-0.595E 00	0.163E-02
1.541	0.491E 02	0.138E-01	0.253E 02	0.953E-01	-0.329E 00	-0.507E 00	0.203E-02
1.618	0.477E 02	0.143E-01	0.312E 02	0.108E 00	-0.235E 00	-0.380E 00	0.249E-02
1.695	0.464E 02	0.147E-01	0.385E 02	0.126E 00	-0.116E 00	-0.197E 00	0.263E-02
1.771	0.450E 02	0.152E-01	0.457E 02	0.125E 00	0.108E-01	0.191E-01	0.336E-02
1.848	0.436E 02	0.157E-01	0.523E 02	0.142E 00	0.137E 00	0.253E 00	0.414E-02
1.925	0.422E 02	0.163E-01	0.568E 02	0.154E 00	0.238E 00	0.458E 00	0.484E-02
2.002	0.408E 02	0.169E-01	0.577E 02	0.157E 00	0.286E 00	0.572E 00	0.532E-02
2.078	0.395E 02	0.175E-01	0.564E 02	0.154E 00	0.297E 00	0.616E 00	0.562E-02
2.155	0.382E 02	0.182E-01	0.521E 02	0.146E 00	0.271E 00	0.583E 00	0.572E-02
2.231	0.369E 02	0.189E-01	0.497E 02	0.137E 00	0.241E 00	0.538E 00	0.579E-02
2.308	0.356E 02	0.196E-01	0.463E 02	0.129E 00	0.209E 00	0.483E 00	0.585E-02

H_2O 20°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
2.384	0.343E 02	0.204E-01	0.436E 02	0.122E 00	0.189E 00	0.452E 00	0.597E-02
2.461	0.331E 02	0.213E-01	0.416E 02	0.118E 00	0.181E 00	0.445E 00	0.616E-02
2.537	0.319E 02	0.222E-01	0.400E 02	0.114E 00	0.180E 00	0.456E 00	0.640E-02
2.614	0.307E 02	0.231E-01	0.391E 02	0.112E 00	0.193E 00	0.505E 00	0.673E-02
2.690	0.296E 02	0.241E-01	0.390E 02	0.111E 00	0.226E 00	0.607E 00	0.721E-02
2.766	0.285E 02	0.251E-01	0.385E 02	0.110E 00	0.250E 00	0.692E 00	0.765E-02
2.842	0.274E 02	0.261E-01	0.383E 02	0.110E 00	0.284E 00	0.806E 00	0.818E-02
2.918	0.264E 02	0.273E-01	0.368E 02	0.106E 00	0.283E 00	0.825E 00	0.846E-02
2.994	0.254E 02	0.284E-01	0.344E 02	0.100E 00	0.256E 00	0.767E 00	0.855E-02
3.070	0.244E 02	0.297E-01	0.312E 02	0.921E-01	0.200E 00	0.613E 00	0.839E-02
3.146	0.235E 02	0.310E-01	0.273E 02	0.823E-01	0.119E 00	0.375E 00	0.802E-02
3.222	0.226E 02	0.323E-01	0.236E 02	0.727E-01	0.319E-01	0.103E 00	0.757E-02
3.298	0.217E 02	0.338E-01	0.204E 02	0.646E-01	-0.440E-01	-0.145E 00	0.719E-02
3.374	0.209E 02	0.353E-01	0.177E 02	0.576E-01	-0.113E 00	-0.380E 00	0.685E-02
3.450	0.200E 02	0.369E-01	0.158E 02	0.529E-01	-0.155E 00	-0.534E 00	0.673E-02
3.525	0.193E 02	0.385E-01	0.143E 02	0.491E-01	-0.189E 00	-0.667E 00	0.666E-02
3.601	0.185E 02	0.402E-01	0.134E 02	0.467E-01	-0.205E 00	-0.739E 00	0.676E-02
3.676	0.178E 02	0.420E-01	0.127E 02	0.452E-01	-0.213E 00	-0.782E 00	0.699E-02
3.752	0.171E 02	0.439E-01	0.124E 02	0.441E-01	-0.207E 00	-0.777E 00	0.726E-02
3.827	0.164E 02	0.458E-01	0.122E 02	0.438E-01	-0.192E 00	-0.735E 00	0.768E-02
3.902	0.158E 02	0.478E-01	0.122E 02	0.437E-01	-0.174E 00	-0.677E 00	0.814E-02
3.978	0.152E 02	0.498E-01	0.122E 02	0.438E-01	-0.149E 00	-0.591E 00	0.868E-02
4.053	0.146E 02	0.520E-01	0.122E 02	0.438E-01	-0.126E 00	-0.509E 00	0.923E-02
4.128	0.141E 02	0.543E-01	0.124E 02	0.441E-01	-0.929E-01	-0.384E 00	0.988E-02
4.203	0.135E 02	0.566E-01	0.123E 02	0.441E-01	-0.683E-01	-0.287E 00	0.105E-01
4.278	0.130E 02	0.591E-01	0.124E 02	0.440E-01	-0.406E-01	-0.174E 00	0.111E-01
4.427	0.121E 02	0.641E-01	0.122E 02	0.253E-01	0.683E-02	0.303E-01	0.718E-02
4.576	0.113E 02	0.694E-01	0.119E 02	0.248E-01	0.429E-01	0.196E 00	0.788E-02
4.725	0.105E 02	0.753E-01	0.113E 02	0.239E-01	0.587E-01	0.277E 00	0.849E-02
4.874	0.975E 01	0.814E-01	0.105E 02	0.228E-01	0.633E-01	0.308E 00	0.905E-02
5.022	0.911E 01	0.877E-01	0.968E 01	0.215E-01	0.499E-01	0.251E 00	0.949E-02
5.170	0.851E 01	0.946E-01	0.876E 01	0.201E-01	0.237E-01	0.123E 00	0.985E-02
5.317	0.797E 01	0.102E 00	0.788E 01	0.189E-01	-0.912E-02	-0.485E-01	0.102E-01
5.464	0.750E 01	0.109E 00	0.710E 01	0.176E-01	-0.437E-01	-0.239E 00	0.105E-01
5.610	0.705E 01	0.117E 00	0.643E 01	0.166E-01	-0.732E-01	-0.411E 00	0.108E-01
5.757	0.665E 01	0.125E 00	0.590E 01	0.157E-01	-0.930E-01	-0.535E 00	0.113E-01
5.902	0.628E 01	0.133E 00	0.546E 01	0.151E-01	-0.109E 00	-0.641E 00	0.118E-01
6.047	0.595E 01	0.141E 00	0.524E 01	0.147E-01	-0.100E 00	-0.606E 00	0.125E-01
6.192	0.564E 01	0.150E 00	0.512E 01	0.144E-01	-0.784E-01	-0.485E 00	0.133E-01
6.337	0.536E 01	0.159E 00	0.507E 01	0.142E-01	-0.465E-01	-0.294E 00	0.143E-01
6.480	0.511E 01	0.167E 00	0.504E 01	0.141E-01	-0.115E-01	-0.748E-01	0.153E-01
6.624	0.488E 01	0.176E 00	0.500E 01	0.140E-01	0.216E-01	0.143E 00	0.163E-01
6.766	0.466E 01	0.186E 00	0.494E 01	0.138E-01	0.511E-01	0.346E 00	0.173E-01
6.909	0.447E 01	0.194E 00	0.482E 01	0.135E-01	0.680E-01	0.470E 00	0.182E-01
7.051	0.430E 01	0.203E 00	0.472E 01	0.133E-01	0.863E-01	0.609E 00	0.191E-01
7.192	0.413E 01	0.213E 00	0.460E 01	0.130E-01	0.779E-01	0.561E 00	0.199E-01
7.332	0.398E 01	0.222E 00	0.424E 01	0.124E-01	0.579E-01	0.425E 00	0.205E-01
7.473	0.384E 01	0.231E 00	0.399E 01	0.122E-01	0.327E-01	0.244E 00	0.210E-01
7.612	0.372E 01	0.240E 00	0.377E 01	0.118E-01	0.125E-01	0.951E-01	0.215E-01
7.751	0.360E 01	0.249E 00	0.355E 01	0.113E-01	-0.109E-01	-0.845E-01	0.219E-01
7.890	0.349E 01	0.258E 00	0.340E 01	0.110E-01	-0.239E-01	-0.188E 00	0.223E-01
8.027	0.339E 01	0.266E 00	0.328E 01	0.107E-01	-0.301E-01	-0.242E 00	0.228E-01
8.164	0.329E 01	0.275E 00	0.316E 01	0.104E-01	-0.368E-01	-0.301E 00	0.234E-01
8.301	0.321E 01	0.284E 00	0.310E 01	0.102E-01	-0.392E-01	-0.343E 00	0.240E-01
8.437	0.313E 01	0.292E 00	0.304E 01	0.100E-01	-0.240E-01	-0.202E 00	0.247E-01
8.572	0.305E 01	0.300E 00	0.299E 01	0.984E-02	-0.170E-01	-0.146E 00	0.253E-01
8.707	0.298E 01	0.309E 00	0.298E 01	0.973E-02	-0.535E-03	-0.466E-02	0.261E-01
8.841	0.291E 01	0.317E 00	0.295E 01	0.960E-02	0.105E-01	0.931E-01	0.269E-01
8.974	0.285E 01	0.324E 00	0.292E 01	0.949E-02	0.225E-01	0.202E 00	0.276E-01
9.107	0.279E 01	0.332E 00	0.289E 01	0.935E-02	0.304E-01	0.277E 00	0.283E-01
9.239	0.274E 01	0.340E 00	0.282E 01	0.919E-02	0.291E-01	0.269E 00	0.289E-01
9.370	0.269E 01	0.347E 00	0.279E 01	0.907E-02	0.361E-01	0.338E 00	0.295E-01
9.500	0.264E 01	0.355E 00	0.272E 01	0.889E-02	0.274E-01	0.260E 00	0.300E-01
9.630	0.259E 01	0.362E 00	0.265E 01	0.871E-02	0.190E-01	0.183E 00	0.304E-01
9.759	0.255E 01	0.369E 00	0.258E 01	0.854E-02	0.111E-01	0.109E 00	0.307E-01
9.887	0.251E 01	0.376E 00	0.250E 01	0.835E-02	-0.896E-02	-0.886E-02	0.310E-01
10.015	0.247E 01	0.382E 00	0.245E 01	0.819E-02	-0.633E-02	-0.634E-01	0.314E-01
10.142	0.243E 01	0.389E 00	0.237E 01	0.799E-02	-0.216E-01	-0.219E 00	0.315E-01
10.268	0.239E 01	0.396E 00	0.234E 01	0.786E-02	-0.199E-01	-0.204E 00	0.320E-01
10.393	0.236E 01	0.403E 00	0.230E 01	0.771E-02	-0.246E-01	-0.256E 00	0.322E-01
10.517	0.233E 01	0.409E 00	0.227E 01	0.759E-02	-0.207E-01	-0.218E 00	0.327E-01
10.641	0.229E 01	0.416E 00	0.226E 01	0.750E-02	-0.157E-01	-0.167E 00	0.332E-01
10.764	0.226E 01	0.422E 00	0.222E 01	0.737E-02	-0.187E-01	-0.201E 00	0.335E-01
10.886	0.224E 01	0.429E 00	0.222E 01	0.730E-02	-0.825E-02	-0.898E-01	0.341E-01
11.007	0.221E 01	0.435E 00	0.220E 01	0.719E-02	-0.400E-02	-0.440E-01	0.345E-01
11.127	0.218E 01	0.442E 00	0.218E 01	0.712E-02	0.162E-02	0.181E-01	0.350E-01

H_2O 20°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
11.247	0.215E 01	0.448E 00	0.217E 01	0.709E-02	0.913E-02	0.103E 00	0.356E-01
11.366	0.213E 01	0.454E 00	0.215E 01	0.699E-02	0.887E-02	0.101E 00	0.361E-01
11.483	0.210E 01	0.460E 00	0.213E 01	0.554E-02	0.137E-01	0.157E 00	0.293E-01
11.600	0.209E 01	0.466E 00	0.211E 01	0.547E-02	0.135E-01	0.157E 00	0.295E-01
11.716	0.206E 01	0.472E 00	0.207E 01	0.538E-02	0.781E-02	0.915E-01	0.297E-01
11.831	0.203E 01	0.477E 00	0.205E 01	0.532E-02	0.911E-02	0.108E 00	0.300E-01
11.946	0.201E 01	0.483E 00	0.203E 01	0.525E-02	0.109E-01	0.130E 00	0.303E-01
12.059	0.199E 01	0.488E 00	0.200E 01	0.517E-02	0.497E-02	0.599E-01	0.305E-01
12.171	0.197E 01	0.494E 00	0.199E 01	0.512E-02	0.877E-02	0.107E 00	0.308E-01
12.283	0.195E 01	0.499E 00	0.195E 01	0.503E-02	-0.762E-03	-0.936E-02	0.309E-01
12.393	0.193E 01	0.505E 00	0.192E 01	0.497E-02	-0.347E-02	-0.430E-01	0.311E-01
12.503	0.191E 01	0.510E 00	0.190E 01	0.490E-02	-0.681E-02	-0.851E-01	0.313E-01
12.611	0.189E 01	0.516E 00	0.186E 01	0.483E-02	-0.137E-01	-0.173E 00	0.314E-01
12.719	0.187E 01	0.522E 00	0.184E 01	0.476E-02	-0.169E-01	-0.215E 00	0.316E-01
12.826	0.185E 01	0.528E 00	0.183E 01	0.472E-02	-0.120E-01	-0.154E 00	0.319E-01
12.932	0.183E 01	0.534E 00	0.181E 01	0.467E-02	-0.106E-01	-0.137E 00	0.322E-01
13.036	0.181E 01	0.540E 00	0.180E 01	0.461E-02	-0.977E-02	-0.127E 00	0.325E-01
13.140	0.179E 01	0.546E 00	0.178E 01	0.456E-02	-0.975E-02	-0.128E 00	0.327E-01
13.242	0.178E 01	0.552E 00	0.176E 01	0.451E-02	-0.788E-02	-0.104E 00	0.330E-01
13.345	0.176E 01	0.558E 00	0.175E 01	0.447E-02	-0.219E-02	-0.292E-01	0.333E-01
13.445	0.174E 01	0.565E 00	0.173E 01	0.441E-02	-0.277E-02	-0.372E-01	0.335E-01
13.545	0.172E 01	0.571E 00	0.174E 01	0.439E-02	0.759E-02	0.103E 00	0.339E-01
13.644	0.170E 01	0.577E 00	0.172E 01	0.435E-02	0.101E-01	0.138E 00	0.342E-01
13.741	0.169E 01	0.583E 00	0.170E 01	0.430E-02	0.721E-02	0.991E-01	0.344E-01
13.838	0.167E 01	0.589E 00	0.169E 01	0.426E-02	0.102E-01	0.141E 00	0.347E-01
13.933	0.165E 01	0.595E 00	0.167E 01	0.422E-02	0.119E-01	0.165E 00	0.350E-01
14.028	0.164E 01	0.600E 00	0.165E 01	0.417E-02	0.860E-02	0.121E 00	0.352E-01
14.121	0.162E 01	0.606E 00	0.164E 01	0.414E-02	0.112E-01	0.158E 00	0.354E-01
14.214	0.160E 01	0.612E 00	0.161E 01	0.409E-02	0.432E-02	0.614E-01	0.356E-01
14.305	0.159E 01	0.617E 00	0.160E 01	0.406E-02	0.753E-02	0.108E 00	0.359E-01
14.395	0.158E 01	0.623E 00	0.159E 01	0.402E-02	0.689E-02	0.992E-01	0.361E-01
14.484	0.156E 01	0.628E 00	0.157E 01	0.398E-02	0.339E-02	0.491E-01	0.362E-01
14.572	0.155E 01	0.634E 00	0.156E 01	0.395E-02	0.478E-02	0.696E-01	0.365E-01
14.659	0.154E 01	0.639E 00	0.153E 01	0.390E-02	-0.212E-02	-0.310E-01	0.365E-01
14.744	0.152E 01	0.645E 00	0.152E 01	0.387E-02	-0.168E-02	-0.247E-01	0.367E-01
14.829	0.151E 01	0.650E 00	0.151E 01	0.383E-02	-0.321E-02	-0.476E-01	0.369E-01
14.913	0.150E 01	0.656E 00	0.150E 01	0.380E-02	-0.671E-03	-0.100E-01	0.372E-01
14.995	0.149E 01	0.662E 00	0.148E 01	0.376E-02	-0.572E-02	-0.859E-01	0.373E-01
15.076	0.148E 01	0.668E 00	0.146E 01	0.371E-02	-0.103E-01	-0.155E 00	0.374E-01
15.156	0.147E 01	0.673E 00	0.146E 01	0.369E-02	-0.430E-02	-0.652E-01	0.377E-01
15.235	0.145E 01	0.679E 00	0.144E 01	0.365E-02	-0.897E-02	-0.137E 00	0.377E-01
15.313	0.144E 01	0.685E 00	0.143E 01	0.361E-02	-0.106E-01	-0.162E 00	0.379E-01
15.389	0.143E 01	0.691E 00	0.141E 01	0.358E-02	-0.113E-01	-0.174E 00	0.380E-01
15.465	0.142E 01	0.697E 00	0.141E 01	0.355E-02	-0.737E-02	-0.114E 00	0.382E-01
15.539	0.140E 01	0.702E 00	0.140E 01	0.353E-02	-0.113E-02	-0.176E-01	0.385E-01
15.612	0.139E 01	0.707E 00	0.139E 01	0.350E-02	-0.422E-02	-0.659E-01	0.386E-01
15.684	0.138E 01	0.713E 00	0.139E 01	0.347E-02	-0.286E-02	-0.449E-01	0.388E-01
15.754	0.137E 01	0.719E 00	0.138E 01	0.345E-02	0.209E-02	0.330E-01	0.390E-01
15.824	0.136E 01	0.723E 00	0.137E 01	0.343E-02	0.588E-02	0.930E-01	0.392E-01
15.892	0.135E 01	0.728E 00	0.136E 01	0.340E-02	0.401E-02	0.637E-01	0.393E-01
15.959	0.135E 01	0.732E 00	0.136E 01	0.338E-02	0.774E-02	0.124E 00	0.395E-01
16.025	0.134E 01	0.737E 00	0.135E 01	0.335E-02	0.984E-02	0.158E 00	0.395E-01

RADIAL DISTRIBUTION FUNCTIONS TO 10 A

H_2O 20°C

R	G(R)	R	G(R)	R	G(R)	R	G(R)
0.0	0.0	3.50	0.1201	5.00	0.9873	7.50	0.9960
0.05	-0.2748	3.55	0.2579	5.05	0.9896	7.55	0.9913
0.10	-0.2047	3.60	0.5541	5.10	0.9833	7.60	0.9884
0.15	-0.1133	3.65	0.9746	5.15	0.9857	7.65	0.9862
0.20	-0.0273	3.70	1.4334	5.20	0.9868	7.70	0.9843
0.25	0.0342	3.75	1.8430	5.25	0.9898	7.75	0.9834
0.30	0.0679	3.80	2.1183	5.30	0.9933	7.80	0.9843
0.35	0.0871	3.85	2.2046	5.35	0.9921	7.85	0.9870
0.40	0.1160	3.90	2.1186	5.40	0.9938	7.90	0.9903
0.45	0.1797	3.95	1.9143	5.45	0.9953	7.95	0.9923
0.50	0.2942	4.00	1.6646	5.50	0.9977	8.00	0.9915
0.55	0.4608	4.05	1.4334	5.55	0.9971	8.05	0.9876
0.60	0.6666	4.10	1.2561	5.60	0.9966	8.10	0.9822
0.65	0.8908	4.15	1.1361	5.65	0.9901	8.15	0.9781
0.70	1.1111	4.20	1.0550	5.70	0.9957	8.20	0.9776
0.75	1.3099	4.25	0.9899	5.75	0.9965	8.25	0.9816
0.80	1.4744	4.30	0.9278	5.80	0.8998	8.30	0.9885

H_2O 20°C

R	G(R)	R	G(R)	R	G(R)	R	G(R)
0.85	1.5951	3.35	0.8714	5.85	0.9003	8.35	0.9953
0.90	1.6619	3.40	0.8334	5.90	0.9102	8.40	0.9989
0.95	1.6632	3.45	0.8266	5.95	0.9268	8.45	0.9978
1.00	1.5391	3.50	0.8533	6.00	0.9449	8.50	0.9929
1.05	1.4375	3.55	0.9029	6.05	0.9594	8.55	0.9871
1.10	1.2200	3.60	0.9559	6.10	0.9685	8.60	0.9838
1.15	0.9629	3.65	0.9941	6.15	0.9740	8.65	0.9850
1.20	0.7026	3.70	1.0082	6.20	0.9800	8.70	0.9907
1.25	0.4752	3.75	1.0016	6.25	0.9899	8.75	0.9986
1.30	0.3049	3.80	0.9868	6.30	1.0042	8.80	1.0055
1.35	0.1969	3.85	0.9778	6.35	1.0201	8.85	1.0089
1.40	0.1380	3.90	0.9823	6.40	1.0330	8.90	1.0084
1.45	0.1050	3.95	0.9992	6.45	1.0393	8.95	1.0051
1.50	0.0775	4.00	1.0207	6.50	1.0388	9.00	1.0015
1.55	0.0476	4.05	1.0373	6.55	1.0345	9.05	0.9997
1.60	0.0226	4.10	1.0443	6.60	1.0312	9.10	1.0005
1.65	0.0188	4.15	1.0432	6.65	1.0328	9.15	1.0030
1.70	0.0497	4.20	1.0406	6.70	1.0400	9.20	1.0054
1.75	0.1150	4.25	1.0428	6.75	1.0502	9.25	1.0061
1.80	0.1978	4.30	1.0525	6.80	1.0587	9.30	1.0046
1.85	0.2706	4.35	1.0670	6.85	1.0615	9.35	1.0013
1.90	0.3087	4.40	1.0809	6.90	1.0575	9.40	0.9978
1.95	0.3032	4.45	1.0892	6.95	1.0488	9.45	0.9953
2.00	0.2670	4.50	1.0915	7.00	1.0398	9.50	0.9946
2.05	0.2283	4.55	1.0911	7.05	1.0343	9.55	0.9953
2.10	0.2162	4.60	1.0930	7.10	1.0339	9.60	0.9966
2.15	0.2434	4.65	1.1000	7.15	1.0370	9.65	0.9977
2.20	0.2975	4.70	1.1098	7.20	1.0403	9.70	0.9982
2.25	0.3457	4.75	1.1157	7.25	1.0401	9.75	0.9982
2.30	0.3519	4.80	1.1103	7.30	1.0349	9.80	0.9982
2.35	0.2990	4.85	1.0897	7.35	1.0253	9.85	0.9985
2.40	0.2047	4.90	1.0565	7.40	1.0139	9.90	0.9992
2.45	0.1218	4.95	1.0190	7.45	1.0036	9.95	0.9998

INTENSITIES IN ELECTRON UNITS H_2O 25°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
0.0	0.660E 02	0.100E-01	0.621E 01	0.600E-01	-0.598E 00	0.0	0.0
0.100	0.659E 02	0.100E-01	0.621E 01	0.600E-01	-0.598E 00	-0.598E-01	0.601E-04
0.200	0.656E 02	0.101E-01	0.621E 01	0.600E-01	-0.598E 00	-0.120E 00	0.121E-03
0.300	0.652E 02	0.101E-01	0.621E 01	0.600E-01	-0.598E 00	-0.179E 00	0.183E-03
0.400	0.646E 02	0.102E-01	0.621E 01	0.600E-01	-0.598E 00	-0.239E 00	0.246E-03
0.500	0.638E 02	0.104E-01	0.621E 01	0.600E-01	-0.598E 00	-0.299E 00	0.311E-03
0.533	0.636E 02	0.104E-01	0.626E 01	0.599E-01	-0.597E 00	-0.319E 00	0.333E-03
0.633	0.626E 02	0.106E-01	0.656E 01	0.596E-01	-0.594E 00	-0.376E 00	0.400E-03
0.733	0.616E 02	0.108E-01	0.709E 01	0.590E-01	-0.588E 00	-0.431E 00	0.467E-03
0.833	0.603E 02	0.110E-01	0.784E 01	0.581E-01	-0.579E 00	-0.483E 00	0.535E-03
0.933	0.589E 02	0.113E-01	0.882E 01	0.570E-01	-0.567E 00	-0.530E 00	0.602E-03
1.033	0.575E 02	0.116E-01	0.100E 02	0.556E-01	-0.552E 00	-0.571E 00	0.669E-03
1.133	0.560E 02	0.120E-01	0.115E 02	0.540E-01	-0.533E 00	-0.604E 00	0.733E-03
1.233	0.544E 02	0.124E-01	0.131E 02	0.521E-01	-0.510E 00	-0.629E 00	0.794E-03
1.310	0.531E 02	0.127E-01	0.154E 02	0.508E-01	-0.479E 00	-0.627E 00	0.101E-02
1.387	0.518E 02	0.130E-01	0.184E 02	0.721E-01	-0.435E 00	-0.604E 00	0.130E-02
1.464	0.504E 02	0.134E-01	0.226E 02	0.875E-01	-0.373E 00	-0.546E 00	0.172E-02
1.541	0.491E 02	0.138E-01	0.278E 02	0.106E 00	-0.294E 00	-0.453E 00	0.227E-02
1.618	0.477E 02	0.142E-01	0.339E 02	0.129E 00	-0.197E 00	-0.318E 00	0.297E-02
1.695	0.464E 02	0.147E-01	0.413E 02	0.155E 00	-0.754E-01	-0.128E 00	0.387E-02
1.771	0.450E 02	0.152E-01	0.484E 02	0.181E 00	0.520E-01	0.922E-01	0.488E-02
1.848	0.436E 02	0.157E-01	0.546E 02	0.203E 00	0.172E 00	0.318E 00	0.592E-02
1.925	0.422E 02	0.163E-01	0.577E 02	0.215E 00	0.251E 00	0.484E 00	0.675E-02
2.002	0.408E 02	0.169E-01	0.588E 02	0.220E 00	0.305E 00	0.611E 00	0.744E-02
2.078	0.395E 02	0.175E-01	0.564E 02	0.212E 00	0.296E 00	0.615E 00	0.771E-02
2.155	0.382E 02	0.182E-01	0.532E 02	0.201E 00	0.272E 00	0.587E 00	0.787E-02
2.231	0.369E 02	0.189E-01	0.491E 02	0.187E 00	0.230E 00	0.513E 00	0.788E-02
2.308	0.356E 02	0.196E-01	0.457E 02	0.175E 00	0.197E 00	0.455E 00	0.795E-02
2.384	0.343E 02	0.204E-01	0.428E 02	0.166E 00	0.173E 00	0.414E 00	0.808E-02
2.461	0.331E 02	0.213E-01	0.405E 02	0.158E 00	0.157E 00	0.386E 00	0.828E-02
2.537	0.319E 02	0.222E-01	0.391E 02	0.153E 00	0.160E 00	0.406E 00	0.864E-02
2.614	0.307E 02	0.231E-01	0.387E 02	0.152E 00	0.184E 00	0.480E 00	0.918E-02
2.690	0.296E 02	0.241E-01	0.381E 02	0.150E 00	0.204E 00	0.549E 00	0.971E-02
2.766	0.285E 02	0.251E-01	0.376E 02	0.149E 00	0.229E 00	0.633E 00	0.103E-01
2.842	0.274E 02	0.261E-01	0.369E 02	0.146E 00	0.247E 00	0.702E 00	0.108E-01

H_2O 25°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
2.918	0.264E 02	0.273E-01	0.349E 02	0.139E 00	0.232E 00	0.678E 00	0.111E-01
2.964	0.254E 02	0.284E-01	0.321E 02	0.129E 00	0.192E 00	0.574E 00	0.110E-01
3.070	0.244E 02	0.297E-01	0.287E 02	0.119E 00	0.128E 00	0.392E 00	0.109E-01
3.146	0.235E 02	0.310E-01	0.255E 02	0.106E 00	0.624E-01	0.196E 00	0.103E-01
3.222	0.226E 02	0.323E-01	0.215E 02	0.928E-01	-0.363E-01	-0.117E 00	0.968E-02
3.298	0.217E 02	0.338E-01	0.190E 02	0.828E-01	-0.907E-01	-0.299E 00	0.922E-02
3.374	0.209E 02	0.353E-01	0.163E 02	0.734E-01	-0.161E 00	-0.545E 00	0.873E-02
3.450	0.200E 02	0.369E-01	0.145E 02	0.668E-01	-0.203E 00	-0.700E 00	0.850E-02
3.525	0.193E 02	0.385E-01	0.135E 02	0.622E-01	-0.223E 00	-0.788E 00	0.844E-02
3.601	0.185E 02	0.402E-01	0.124E 02	0.589E-01	-0.247E 00	-0.889E 00	0.853E-02
3.676	0.178E 02	0.420E-01	0.122E 02	0.568E-01	-0.235E 00	-0.865E 00	0.877E-02
3.827	0.164E 02	0.458E-01	0.121E 02	0.421E-01	-0.197E 00	-0.755E 00	0.738E-02
3.978	0.152E 02	0.499E-01	0.121E 02	0.419E-01	-0.155E 00	-0.615E 00	0.830E-02
4.128	0.141E 02	0.543E-01	0.123E 02	0.420E-01	-0.978E-01	-0.403E 00	0.941E-02
4.278	0.130E 02	0.591E-01	0.124E 02	0.419E-01	-0.402E-01	-0.172E 00	0.106E-01
4.427	0.121E 02	0.641E-01	0.122E 02	0.412E-01	0.611E-02	0.271E-01	0.117E-01
4.576	0.113E 02	0.694E-01	0.117E 02	0.395E-01	0.274E-01	0.125E 00	0.126E-01
4.725	0.105E 02	0.753E-01	0.112E 02	0.380E-01	0.513E-01	0.243E 00	0.135E-01
4.874	0.975E 01	0.814E-01	0.104E 02	0.358E-01	0.519E-01	0.253E 00	0.142E-01
5.022	0.911E 01	0.877E-01	0.950E 01	0.333E-01	0.349E-01	0.175E 00	0.147E-01
5.170	0.851E 01	0.946E-01	0.860E 01	0.306E-01	0.859E-02	0.444E-01	0.150E-01
5.317	0.797E 01	0.102E 00	0.776E 01	0.281E-01	-0.213E-01	-0.113E 00	0.152E-01
5.464	0.750E 01	0.109E 00	0.708E 01	0.260E-01	-0.458E-01	-0.250E 00	0.155E-01
5.610	0.705E 01	0.117E 00	0.636E 01	0.238E-01	-0.808E-01	-0.453E 00	0.156E-01
5.757	0.665E 01	0.125E 00	0.585E 01	0.222E-01	-0.993E-01	-0.572E 00	0.159E-01
5.902	0.628E 01	0.133E 00	0.546E 01	0.209E-01	-0.109E 00	-0.642E 00	0.164E-01
6.047	0.595E 01	0.141E 00	0.527E 01	0.201E-01	-0.964E-01	-0.583E 00	0.171E-01
6.192	0.564E 01	0.150E 00	0.516E 01	0.194E-01	-0.724E-01	-0.448E 00	0.180E-01
6.337	0.536E 01	0.158E 00	0.510E 01	0.188E-01	-0.412E-01	-0.261E 00	0.189E-01
6.480	0.511E 01	0.167E 00	0.506E 01	0.183E-01	-0.872E-02	-0.565E-01	0.198E-01
6.624	0.488E 01	0.176E 00	0.497E 01	0.178E-01	0.156E-01	0.103E 00	0.207E-01
6.766	0.466E 01	0.185E 00	0.494E 01	0.174E-01	0.507E-01	0.343E 00	0.218E-01
6.909	0.447E 01	0.194E 00	0.482E 01	0.168E-01	0.677E-01	0.468E 00	0.225E-01
7.051	0.430E 01	0.203E 00	0.467E 01	0.161E-01	0.767E-01	0.541E 00	0.231E-01
7.192	0.413E 01	0.213E 00	0.446E 01	0.153E-01	0.693E-01	0.499E 00	0.234E-01
7.332	0.398E 01	0.222E 00	0.428E 01	0.146E-01	0.655E-01	0.481E 00	0.237E-01
7.473	0.384E 01	0.231E 00	0.401E 01	0.138E-01	0.378E-01	0.282E 00	0.238E-01
7.612	0.372E 01	0.240E 00	0.379E 01	0.129E-01	0.167E-01	0.127E 00	0.236E-01
7.751	0.360E 01	0.249E 00	0.358E 01	0.122E-01	-0.535E-02	-0.415E-01	0.235E-01
7.890	0.349E 01	0.258E 00	0.339E 01	0.114E-01	-0.244E-01	-0.192E 00	0.232E-01
8.027	0.339E 01	0.266E 00	0.328E 01	0.109E-01	-0.305E-01	-0.245E 00	0.233E-01
8.164	0.329E 01	0.275E 00	0.314E 01	0.103E-01	-0.420E-01	-0.343E 00	0.232E-01
8.301	0.321E 01	0.284E 00	0.307E 01	0.995E-02	-0.380E-01	-0.316E 00	0.234E-01
8.437	0.313E 01	0.292E 00	0.303E 01	0.960E-02	-0.269E-01	-0.227E 00	0.237E-01
8.572	0.305E 01	0.300E 00	0.301E 01	0.819E-02	-0.117E-01	-0.101E 00	0.211E-01
8.707	0.298E 01	0.309E 00	0.299E 01	0.802E-02	0.311E-02	0.271E-01	0.215E-01
8.841	0.291E 01	0.317E 00	0.294E 01	0.779E-02	0.904E-02	0.799E-01	0.218E-01
8.974	0.285E 01	0.324E 00	0.292E 01	0.764E-02	0.230E-01	0.207E 00	0.222E-01
9.107	0.279E 01	0.332E 00	0.288E 01	0.745E-02	0.280E-01	0.255E 00	0.225E-01
9.239	0.274E 01	0.340E 00	0.283E 01	0.726E-02	0.303E-01	0.280E 00	0.228E-01
9.370	0.269E 01	0.347E 00	0.278E 01	0.707E-02	0.314E-01	0.294E 00	0.230E-01
9.500	0.264E 01	0.355E 00	0.271E 01	0.685E-02	0.265E-01	0.251E 00	0.231E-01
9.630	0.259E 01	0.362E 00	0.266E 01	0.667E-02	0.230E-01	0.222E 00	0.232E-01
9.759	0.255E 01	0.369E 00	0.259E 01	0.646E-02	0.146E-01	0.142E 00	0.233E-01
9.887	0.251E 01	0.376E 00	0.251E 01	0.624E-02	0.222E-02	0.220E-01	0.232E-01
10.015	0.247E 01	0.382E 00	0.244E 01	0.604E-02	-0.877E-02	-0.878E-01	0.231E-01
10.142	0.243E 01	0.389E 00	0.239E 01	0.588E-02	-0.128E-01	-0.130E 00	0.232E-01
10.268	0.239E 01	0.396E 00	0.234E 01	0.571E-02	-0.201E-01	-0.206E 00	0.232E-01
10.393	0.236E 01	0.403E 00	0.231E 01	0.560E-02	-0.196E-01	-0.204E 00	0.234E-01
10.517	0.233E 01	0.409E 00	0.227E 01	0.544E-02	-0.238E-01	-0.251E 00	0.234E-01
10.641	0.229E 01	0.416E 00	0.225E 01	0.537E-02	-0.192E-01	-0.204E 00	0.237E-01
10.764	0.226E 01	0.422E 00	0.222E 01	0.527E-02	-0.175E-01	-0.188E 00	0.240E-01
10.886	0.224E 01	0.429E 00	0.221E 01	0.464E-02	-0.128E-01	-0.139E 00	0.217E-01
11.007	0.221E 01	0.435E 00	0.220E 01	0.458E-02	-0.576E-02	-0.634E-01	0.220E-01
11.127	0.218E 01	0.442E 00	0.216E 01	0.450E-02	-0.724E-02	-0.805E-01	0.221E-01
11.247	0.215E 01	0.448E 00	0.216E 01	0.447E-02	0.451E-03	0.507E-02	0.225E-01
11.366	0.213E 01	0.454E 00	0.214E 01	0.441E-02	0.421E-02	0.478E-01	0.228E-01
11.483	0.210E 01	0.460E 00	0.213E 01	0.437E-02	0.109E-01	0.126E 00	0.231E-01
11.600	0.208E 01	0.466E 00	0.211E 01	0.432E-02	0.140E-01	0.163E 00	0.234E-01
11.716	0.206E 01	0.472E 00	0.208E 01	0.426E-02	0.124E-01	0.145E 00	0.235E-01
11.831	0.203E 01	0.477E 00	0.206E 01	0.421E-02	0.144E-01	0.171E 00	0.238E-01
11.946	0.201E 01	0.483E 00	0.203E 01	0.414E-02	0.109E-01	0.130E 00	0.239E-01
12.059	0.199E 01	0.488E 00	0.200E 01	0.406E-02	0.393E-02	0.474E-01	0.239E-01
12.171	0.197E 01	0.494E 00	0.198E 01	0.401E-02	0.361E-02	0.439E-01	0.241E-01
12.283	0.195E 01	0.499E 00	0.195E 01	0.395E-02	0.567E-03	0.697E-02	0.242E-01

H_2O 25°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
12.393	0.193E 01	0.505E 00	0.192E 01	0.388E-02	-0.361E-02	-0.447E-01	0.243E-01
12.503	0.191E 01	0.510E 00	0.189E 01	0.382E-02	-0.800E-02	-0.100E 00	0.244E-01
12.611	0.189E 01	0.516E 00	0.188E 01	0.379E-02	-0.648E-02	-0.817E-01	0.247E-01
12.719	0.187E 01	0.522E 00	0.186E 01	0.375E-02	-0.664E-02	-0.845E-01	0.249E-01
12.826	0.185E 01	0.528E 00	0.183E 01	0.370E-02	-0.983E-02	-0.126E 00	0.250E-01
12.932	0.183E 01	0.534E 00	0.181E 01	0.366E-02	-0.102E-01	-0.132E 00	0.253E-01
13.036	0.181E 01	0.540E 00	0.179E 01	0.362E-02	-0.101E-01	-0.132E 00	0.255E-01
13.140	0.179E 01	0.546E 00	0.178E 01	0.360E-02	-0.738E-02	-0.969E-01	0.258E-01
13.243	0.178E 01	0.552E 00	0.177E 01	0.358E-02	-0.143E-02	-0.189E-01	0.262E-01
13.345	0.176E 01	0.559E 00	0.176E 01	0.356E-02	0.287E-03	0.383E-02	0.266E-01
13.445	0.174E 01	0.565E 00	0.174E 01	0.353E-02	0.418E-03	0.563E-02	0.268E-01
13.545	0.172E 01	0.571E 00	0.173E 01	0.351E-02	0.400E-02	0.542E-01	0.272E-01
13.644	0.170E 01	0.577E 00	0.172E 01	0.351E-02	0.719E-02	0.981E-01	0.276E-01
13.838	0.167E 01	0.589E 00	0.169E 01	0.291E-02	0.106E-01	0.147E 00	0.227E-01
14.028	0.164E 01	0.600E 00	0.165E 01	0.285E-02	0.917E-02	0.129E 00	0.240E-01
14.214	0.160E 01	0.612E 00	0.162E 01	0.282E-02	0.103E-01	0.146E 00	0.245E-01
14.395	0.158E 01	0.623E 00	0.159E 01	0.278E-02	0.797E-02	0.115E 00	0.249E-01
14.572	0.155E 01	0.634E 00	0.155E 01	0.273E-02	0.938E-03	0.137E-01	0.252E-01
14.744	0.152E 01	0.645E 00	0.152E 01	0.269E-02	-0.155E-02	-0.228E-01	0.256E-01
14.913	0.150E 01	0.656E 00	0.149E 01	0.265E-02	-0.518E-02	-0.773E-01	0.259E-01
15.076	0.148E 01	0.668E 00	0.147E 01	0.262E-02	-0.742E-02	-0.112E 00	0.264E-01
15.235	0.145E 01	0.679E 00	0.144E 01	0.260E-02	-0.664E-02	-0.101E 00	0.269E-01
15.389	0.143E 01	0.691E 00	0.142E 01	0.257E-02	-0.729E-02	-0.112E 00	0.273E-01
15.539	0.140E 01	0.702E 00	0.140E 01	0.255E-02	-0.445E-02	-0.692E-01	0.279E-01
15.684	0.138E 01	0.713E 00	0.138E 01	0.254E-02	-0.296E-02	-0.464E-01	0.283E-01

RADIAL DISTRIBUTION FUNCTIONS TO 10 A

H_2O 25°C

R	G(R)	R	G(R)	R	G(R)	R	G(R)
0.0	0.0	2.50	0.0231	5.00	1.0237	7.50	1.0074
0.05	-1.5037	2.55	0.1892	5.05	1.0058	7.55	1.0045
0.10	-1.3846	2.60	0.5089	5.10	0.9913	7.60	1.0009
0.15	-1.2315	2.65	0.9387	5.15	0.9806	7.65	0.9961
0.20	-1.0884	2.70	1.3966	5.20	0.9723	7.70	0.9905
0.25	-0.9810	2.75	1.7885	5.25	0.9641	7.75	0.9852
0.30	-0.9045	2.80	2.0296	5.30	0.9541	7.80	0.9816
0.35	-0.8267	2.85	2.1174	5.35	0.9422	7.85	0.9806
0.40	-0.7056	2.90	2.0377	5.40	0.9293	7.90	0.9823
0.45	-0.5111	2.95	1.8531	5.45	0.9174	7.95	0.9857
0.50	-0.2403	3.00	1.6298	5.50	0.9079	8.00	0.9893
0.55	0.0811	3.05	1.4238	5.55	0.9012	8.05	0.9917
0.60	0.4122	3.10	1.2656	5.60	0.8971	8.10	0.9924
0.65	0.7156	3.15	1.1578	5.65	0.8947	8.15	0.9915
0.70	0.9735	3.20	1.0851	5.70	0.8939	8.20	0.9899
0.75	1.1901	3.25	1.0280	5.75	0.8952	8.25	0.9885
0.80	1.3816	3.30	0.9752	5.80	0.8998	8.30	0.9881
0.85	1.5590	3.35	0.9273	5.85	0.9084	8.35	0.9886
0.90	1.7140	3.40	0.8935	5.90	0.9206	8.40	0.9896
0.95	1.8166	3.45	0.8832	5.95	0.9351	8.45	0.9903
1.00	1.8275	3.50	0.8988	6.00	0.9494	8.50	0.9907
1.05	1.7189	3.55	0.9330	6.05	0.9611	8.55	0.9908
1.10	1.4929	3.60	0.9718	6.10	0.9691	8.60	0.9912
1.15	1.1872	3.65	1.0011	6.15	0.9737	8.65	0.9922
1.20	0.8646	3.70	1.0131	6.20	0.9766	8.70	0.9941
1.25	0.5903	3.75	1.0083	6.25	0.9802	8.75	0.9964
1.30	0.4070	3.80	0.9948	6.30	0.9863	8.80	0.9984
1.35	0.3203	3.85	0.9823	6.35	0.9954	8.85	0.9995
1.40	0.3011	3.90	0.9778	6.40	1.0068	8.90	0.9995
1.45	0.3032	3.95	0.9825	6.45	1.0190	8.95	0.9988
1.50	0.2866	4.00	0.9928	6.50	1.0299	9.00	0.9981
1.55	0.2364	4.05	1.0036	6.55	1.0384	9.05	0.9982
1.60	0.1666	4.10	1.0114	6.60	1.0439	9.10	0.9993
1.65	0.1090	4.15	1.0168	6.65	1.0465	9.15	1.0013
1.70	0.0933	4.20	1.0229	6.70	1.0471	9.20	1.0032
1.75	0.1299	4.25	1.0335	6.75	1.0465	9.25	1.0045
1.80	0.2036	4.30	1.0501	6.80	1.0453	9.30	1.0044
1.85	0.2816	4.35	1.0705	6.85	1.0443	9.35	1.0033
1.90	0.3314	4.40	1.0897	6.90	1.0438	9.40	1.0017
1.95	0.3373	4.45	1.1028	6.95	1.0442	9.45	1.0002
2.00	0.3081	4.50	1.1072	7.00	1.0452	9.50	0.9994
2.05	0.2701	4.55	1.1035	7.05	1.0464	9.55	0.9994
2.10	0.2509	4.60	1.0956	7.10	1.0468	9.60	0.9997

H_2O 25°C

R	G(R)	R	G(R)	R	G(R)	R	G(R)
2.15	0.2617	4.65	1.0876	7.15	1.0455	9.65	0.9999
2.20	0.2894	4.70	1.0823	7.20	1.0419	9.70	0.9995
2.25	0.3032	4.75	1.0796	7.25	1.0361	9.75	0.9986
2.30	0.2729	4.80	1.0768	7.30	1.0289	9.80	0.9976
2.35	0.1903	4.85	1.0706	7.35	1.0216	9.85	0.9968
2.40	0.0816	4.90	1.0591	7.40	1.0153	9.90	0.9968
2.45	0.0036	4.95	1.0426	7.45	1.0107	9.95	0.9973

INTENSITIES IN ELECTRON UNITS H_2O 50°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
0.0	0.660E 02	0.100E-01	0.651E C1	0.600E-01	-0.595E 00	0.0	0.0
0.100	0.659E 02	0.100E-01	0.651E C1	0.600E-01	-0.595E C0	-0.595E-01	0.601E-04
0.200	0.656E 02	0.101E-01	0.651E C1	0.600E-01	-0.595E 00	-0.119E 00	0.121E-03
0.300	0.652E 02	0.101E-01	0.651E 01	0.600E-01	-0.595E 00	-0.178E 00	0.183E-03
0.400	0.646E 02	0.102E-01	0.651E C1	0.600E-01	-0.595E C0	-0.238E 00	0.246E-03
0.500	0.638E 02	0.104E-01	0.651E C1	0.600E-01	-0.595E 00	-0.297E 00	0.311E-03
0.533	0.636E 02	0.104E-01	0.660E C1	0.599E-01	-0.594E 00	-0.317E 00	0.333E-03
0.633	0.626E 02	0.106E-01	0.710E C1	0.595E-01	-0.588E 00	-0.373E 00	0.399E-03
0.733	0.616E 02	0.108E-01	0.799E 01	0.589E-01	-0.578E 00	-0.424E 00	0.466E-03
0.833	0.603E 02	0.110E-01	0.927E C1	0.579E-01	-0.563E 00	-0.470E 00	0.532E-03
0.933	0.589E 02	0.113E-01	0.109E 02	0.566E-01	-0.544E 00	-0.507E 00	0.598E-03
1.033	0.575E 02	0.116E-01	0.130E C2	0.551E-01	-0.518E 00	-0.535E 00	0.662E-03
1.133	0.560E 02	0.120E-01	0.154E C2	0.532E-01	-0.486E 00	-0.551E 00	0.723E-03
1.233	0.544E 02	0.124E-01	0.182E 02	0.511E-01	-0.448E 00	-0.552E 00	0.779E-03
1.310	0.531E 02	0.127E-01	0.193E C2	0.545E-01	-0.429E 00	-0.562E 00	0.906E-03
1.387	0.518E 02	0.130E-01	0.227E 02	0.637E-01	-0.379E 00	-0.526E 00	0.115E-02
1.464	0.504E 02	0.134E-01	0.270E 02	0.751E-01	-0.315E 00	-0.462E 00	0.148E-02
1.541	0.491E 02	0.138E-01	0.330E 02	0.913E-01	-0.222E 00	-0.342E 00	0.195E-02
1.618	0.477E 02	0.143E-01	0.386E 02	0.106E 00	-0.130E 00	-0.211E 00	0.245E-02
1.695	0.464E 02	0.147E-01	0.457E C2	0.125E 00	-0.960E-02	-0.163E-01	0.313E-02
1.771	0.450E C2	0.152E-01	0.536E 02	0.147E 00	0.131E 00	0.232E C0	0.395E-02
1.848	0.436E 02	0.157E-01	0.601E C2	0.164E 00	0.260E C0	0.480E C0	0.477E-02
1.925	0.422E 02	0.163E-01	0.647E 02	0.177E C0	0.367E C0	0.706E 00	0.554E-02
2.002	0.408E 02	0.169E-01	0.662E 02	0.181E 00	0.429E C0	0.860E 00	0.614E-02
2.078	0.395E 02	0.175E-01	0.648E 02	0.178E C0	0.443E 00	0.921E 00	0.650E-02
2.155	0.382E 02	0.182E-01	0.622E 02	0.172E 00	0.438E 00	0.943E 00	0.676E-02
2.231	0.369E 02	0.189E-01	0.580E 02	0.162E 00	0.398E 00	0.889E 00	0.684E-02
2.308	0.356E 02	0.196E-01	0.542E 02	0.153E 00	0.366E 00	0.844E 00	0.695E-02
2.384	0.343E 02	0.204E-01	0.504E 02	0.144E 00	0.329E 00	0.785E 00	0.703E-02
2.461	0.331E 02	0.213E-01	0.476E C2	0.138E 00	0.309E 00	0.761E 00	0.722E-02
2.537	0.319E 02	0.222E-01	0.452E C2	0.132E C0	0.296E C0	0.750E 00	0.743E-02
2.614	0.307E 02	0.231E-01	0.435E 02	0.128E 00	0.296E 00	0.774E 00	0.772E-02
2.690	0.296E 02	0.241E-01	0.421E C2	0.124E C0	0.301E 00	0.810E C0	0.806E-02
2.766	0.285E 02	0.251E-01	0.405E 02	0.121E C0	0.300E C0	0.830E C0	0.836E-02
2.842	0.274E 02	0.261E-01	0.382E 02	0.115E C0	0.282E 00	0.801E 00	0.854E-02
2.918	0.264E 02	0.273E-01	0.357E 02	0.109E 00	0.254E 00	0.740E 00	0.865E-02
2.994	0.254E 02	0.284E-01	0.321E 02	0.997E-01	0.191E 00	0.573E 00	0.849E-02
3.070	0.244E 02	0.297E-01	0.280E C2	0.902E-01	0.107E 00	0.328E 00	0.822E-02
3.146	0.235E 02	0.310E-01	0.244E 02	0.800E-01	0.293E-01	0.920E-01	0.780E-02
3.222	0.226E 02	0.323E-01	0.210E 02	0.712E-01	-0.519E-01	-0.167E 00	0.742E-02
3.298	0.217E 02	0.338E-01	0.179E C2	0.632E-01	-0.130E C0	-0.429E 00	0.704E-02
3.374	0.209E 02	0.353E-01	0.157E C2	0.570E-01	-0.181E 00	-0.610E 00	0.679E-02
3.525	0.193E 02	0.385E-01	0.133E 02	0.446E-01	-0.229E C0	-0.807E C0	0.605E-02
3.676	0.178E 02	0.420E-01	0.123E 02	0.418E-01	-0.230E 00	-0.845E 00	0.646E-02
3.827	0.164E 02	0.458E-01	0.120E 02	0.406E-01	-0.202E C0	-0.774E C0	0.712E-02
3.978	0.152E 02	0.499E-01	0.120E C2	0.401E-01	-0.158E 00	-0.630E 00	0.794E-02
4.128	0.141E 02	0.543E-01	0.122E C2	0.399E-01	-0.997E-01	-0.412E 00	0.894E-02
4.278	0.130E 02	0.591E-01	0.123E C2	0.395E-01	-0.413E-01	-0.177E 00	0.998E-02
4.427	0.121E 02	0.641E-01	0.123E 02	0.387E-01	0.938E-02	0.415E-01	0.110E-01
4.576	0.113E 02	0.694E-01	0.119E 02	0.375E-01	0.465E-01	0.213E 00	0.119E-01
4.725	0.105E 02	0.753E-01	0.113E 02	0.357E-01	0.586E-01	0.277E C0	0.127E-01
4.874	0.975E 01	0.814E-01	0.105E 02	0.339E-01	0.638E-01	0.311E 00	0.134E-01
5.022	0.911E 01	0.877E-01	0.960E 01	0.315E-01	0.436E-01	0.219E 00	0.139E-01
5.170	0.851E 01	0.946E-01	0.877E C1	0.294E-01	0.250E-01	0.129E 00	0.144E-01
5.317	0.797E 01	0.102E 00	0.796E 01	0.274E-01	-0.121E-02	-0.645E-02	0.148E-01
5.464	0.750E 01	0.109E 00	0.716E 01	0.254E-01	-0.370E-01	-0.202E C0	0.151E-01
5.610	0.705E 01	0.117E 00	0.655E C1	0.237E-01	-0.593E-01	-0.333E 00	0.155E-01
5.757	0.665E 01	0.125E 00	0.599E 01	0.222E-01	-0.819E-01	-0.472E C0	0.159E-01
5.902	0.628E 01	0.133E 00	0.558E C1	0.210E-01	-0.930E-01	-0.549E 00	0.164E-01
6.047	0.595E 01	0.141E 00	0.523E 01	0.201E-01	-0.102E 00	-0.617E 00	0.171E-01
6.192	0.564E 01	0.150E 00	0.508E C1	0.192E-01	-0.842E-01	-0.522E 00	0.178E-01

H_2O 50°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
6.337	0.536E 01	0.158E 00	0.495E 01	0.185E-01	-0.647E-01	-0.410E 00	0.186E-01
6.480	0.511E 01	0.167E 00	0.501E 01	0.131E-01	-0.174E-01	-0.113E 00	0.142E-01
6.624	0.488E 01	0.176E 00	0.495E 01	0.128E-01	0.132E-01	0.877E-01	0.149E-01
6.766	0.466E 01	0.185E 00	0.493E 01	0.126E-01	0.495E-01	0.335E 00	0.158E-01
6.909	0.447E 01	0.194E 00	0.483E 01	0.122E-01	0.687E-01	0.475E 00	0.164E-01
7.051	0.430E 01	0.203E 00	0.463E 01	0.117E-01	0.678E-01	0.478E 00	0.168E-01
7.192	0.413E 01	0.213E 00	0.449E 01	0.113E-01	0.754E-01	0.542E 00	0.173E-01
7.332	0.398E 01	0.222E 00	0.423E 01	0.108E-01	0.551E-01	0.404E 00	0.175E-01
7.473	0.384E 01	0.231E 00	0.403E 01	0.103E-01	0.426E-01	0.318E 00	0.178E-01
7.612	0.372E 01	0.240E 00	0.383E 01	0.982E-02	0.260E-01	0.198E 00	0.179E-01
7.751	0.360E 01	0.249E 00	0.360E 01	0.932E-02	0.166E-02	0.129E-01	0.180E-01
7.890	0.349E 01	0.258E 00	0.345E 01	0.891E-02	-0.113E-01	-0.892E-01	0.181E-01
8.027	0.339E 01	0.266E 00	0.328E 01	0.849E-02	-0.297E-01	-0.238E 00	0.181E-01
8.164	0.329E 01	0.275E 00	0.318E 01	0.812E-02	-0.329E-01	-0.269E 00	0.182E-01
8.301	0.321E 01	0.284E 00	0.310E 01	0.780E-02	-0.302E-01	-0.251E 00	0.184E-01
8.437	0.313E 01	0.292E 00	0.303E 01	0.750E-02	-0.266E-01	-0.224E 00	0.185E-01
8.572	0.305E 01	0.300E 00	0.298E 01	0.723E-02	-0.198E-01	-0.170E 00	0.186E-01
8.707	0.298E 01	0.309E 00	0.295E 01	0.698E-02	-0.924E-02	-0.804E-01	0.188E-01
8.841	0.291E 01	0.317E 00	0.294E 01	0.678E-02	0.750E-02	0.663E-01	0.190E-01
8.974	0.285E 01	0.324E 00	0.291E 01	0.655E-02	0.194E-01	0.174E 00	0.191E-01
9.107	0.279E 01	0.332E 00	0.288E 01	0.634E-02	0.281E-01	0.256E 00	0.192E-01
9.239	0.274E 01	0.340E 00	0.281E 01	0.609E-02	0.251E-01	0.232E 00	0.191E-01
9.370	0.269E 01	0.347E 00	0.278E 01	0.590E-02	0.335E-01	0.314E 00	0.192E-01
9.500	0.264E 01	0.355E 00	0.272E 01	0.566E-02	0.288E-01	0.273E 00	0.191E-01
9.630	0.259E 01	0.362E 00	0.266E 01	0.546E-02	0.251E-01	0.242E 00	0.190E-01
9.759	0.255E 01	0.369E 00	0.258E 01	0.522E-02	0.111E-01	0.108E 00	0.188E-01
9.887	0.251E 01	0.376E 00	0.251E 01	0.500E-02	0.107E-03	0.106E-02	0.186E-01
10.015	0.247E 01	0.382E 00	0.245E 01	0.481E-02	-0.557E-02	-0.558E-01	0.184E-01
10.142	0.243E 01	0.389E 00	0.238E 01	0.462E-02	-0.184E-01	-0.187E 00	0.182E-01
10.268	0.239E 01	0.396E 00	0.234E 01	0.446E-02	-0.205E-01	-0.210E 00	0.181E-01
10.393	0.236E 01	0.403E 00	0.230E 01	0.429E-02	-0.235E-01	-0.244E 00	0.180E-01
10.517	0.233E 01	0.409E 00	0.227E 01	0.416E-02	-0.224E-01	-0.235E 00	0.179E-01
10.641	0.229E 01	0.416E 00	0.224E 01	0.364E-02	-0.206E-01	-0.220E 00	0.161E-01
10.764	0.226E 01	0.422E 00	0.222E 01	0.356E-02	-0.182E-01	-0.196E 00	0.162E-01
10.886	0.224E 01	0.429E 00	0.221E 01	0.349E-02	-0.116E-01	-0.126E 00	0.163E-01
11.007	0.221E 01	0.435E 00	0.219E 01	0.341E-02	-0.809E-02	-0.890E-01	0.163E-01
11.127	0.218E 01	0.442E 00	0.217E 01	0.335E-02	-0.494E-02	-0.550E-01	0.165E-01
11.247	0.215E 01	0.448E 00	0.215E 01	0.329E-02	-0.195E-02	-0.220E-01	0.166E-01
11.366	0.213E 01	0.454E 00	0.213E 01	0.323E-02	0.487E-03	0.554E-02	0.167E-01
11.483	0.210E 01	0.460E 00	0.212E 01	0.319E-02	0.790E-02	0.908E-01	0.169E-01
11.600	0.208E 01	0.466E 00	0.209E 01	0.313E-02	0.712E-02	0.826E-01	0.169E-01
11.716	0.206E 01	0.472E 00	0.207E 01	0.307E-02	0.789E-02	0.925E-01	0.170E-01
11.831	0.203E 01	0.477E 00	0.204E 01	0.301E-02	0.444E-02	0.525E-01	0.170E-01
11.946	0.201E 01	0.483E 00	0.202E 01	0.296E-02	0.675E-02	0.806E-01	0.171E-01
12.059	0.199E 01	0.488E 00	0.201E 01	0.292E-02	0.968E-02	0.117E 00	0.172E-01
12.171	0.197E 01	0.494E 00	0.198E 01	0.286E-02	0.405E-02	0.492E-01	0.172E-01
12.283	0.195E 01	0.499E 00	0.195E 01	0.282E-02	0.173E-02	0.212E-01	0.173E-01
12.393	0.193E 01	0.505E 00	0.193E 01	0.277E-02	0.400E-04	0.495E-03	0.174E-01
12.503	0.191E 01	0.510E 00	0.190E 01	0.273E-02	-0.231E-02	-0.289E-01	0.174E-01
12.611	0.189E 01	0.516E 00	0.188E 01	0.268E-02	-0.673E-02	-0.849E-01	0.175E-01
12.719	0.187E 01	0.522E 00	0.185E 01	0.264E-02	-0.103E-01	-0.131E 00	0.175E-01
12.826	0.185E 01	0.528E 00	0.184E 01	0.262E-02	-0.819E-02	-0.105E 00	0.177E-01
12.932	0.183E 01	0.534E 00	0.182E 01	0.258E-02	-0.891E-02	-0.115E 00	0.178E-01
13.036	0.181E 01	0.540E 00	0.180E 01	0.255E-02	-0.933E-02	-0.122E 00	0.180E-01
13.140	0.179E 01	0.546E 00	0.178E 01	0.253E-02	-0.712E-02	-0.935E-01	0.182E-01
13.243	0.178E 01	0.552E 00	0.176E 01	0.251E-02	-0.732E-02	-0.969E-01	0.183E-01
13.345	0.176E 01	0.558E 00	0.175E 01	0.248E-02	-0.713E-02	-0.951E-01	0.185E-01
13.445	0.174E 01	0.565E 00	0.173E 01	0.246E-02	-0.637E-02	-0.856E-01	0.187E-01
13.545	0.172E 01	0.571E 00	0.172E 01	0.244E-02	-0.217E-02	-0.293E-01	0.189E-01
13.644	0.170E 01	0.577E 00	0.170E 01	0.242E-02	-0.146E-02	-0.199E-01	0.191E-01
13.741	0.169E 01	0.583E 00	0.169E 01	0.240E-02	0.188E-02	0.259E-01	0.193E-01
13.838	0.167E 01	0.589E 00	0.167E 01	0.238E-02	0.306E-02	0.423E-01	0.194E-01
14.028	0.164E 01	0.600E 00	0.165E 01	0.235E-02	0.836E-02	0.117E 00	0.198E-01
14.214	0.160E 01	0.612E 00	0.162E 01	0.231E-02	0.924E-02	0.131E 00	0.201E-01
14.395	0.158E 01	0.623E 00	0.159E 01	0.226E-02	0.850E-02	0.122E 00	0.203E-01
14.572	0.155E 01	0.634E 00	0.157E 01	0.224E-02	0.112E-01	0.164E 00	0.206E-01
14.744	0.152E 01	0.645E 00	0.153E 01	0.220E-02	0.588E-02	0.867E-01	0.209E-01
14.913	0.150E 01	0.656E 00	0.150E 01	0.216E-02	0.476E-03	0.710E-02	0.211E-01
15.076	0.148E 01	0.668E 00	0.147E 01	0.213E-02	-0.363E-02	-0.548E-01	0.214E-01
15.235	0.145E 01	0.679E 00	0.144E 01	0.210E-02	-0.721E-02	-0.110E 00	0.218E-01
15.389	0.143E 01	0.691E 00	0.141E 01	0.208E-02	-0.105E-01	-0.162E 00	0.221E-01
15.539	0.140E 01	0.702E 00	0.139E 01	0.206E-02	-0.937E-02	-0.146E 00	0.225E-01
15.684	0.138E 01	0.713E 00	0.137E 01	0.204E-02	-0.817E-02	-0.128E 00	0.228E-01
15.824	0.136E 01	0.723E 00	0.135E 01	0.202E-02	-0.626E-02	-0.991E-01	0.231E-01
15.959	0.135E 01	0.732E 00	0.134E 01	0.201E-02	-0.308E-02	-0.491E-01	0.235E-01

RADIAL DISTRIBUTION FUNCTIONS TO 10 A H_2O 50°C

R	G(R)	R	G(R)	R	G(R)	R	G(R)
0.0	0.0	2.50	-0.0961	5.00	0.9975	7.50	1.0089
0.05	-1.5895	2.55	0.1764	5.05	0.9826	7.55	1.0043
0.10	-1.1236	2.60	0.5964	5.10	0.9748	7.60	1.0008
0.15	-0.5046	2.65	1.0853	5.15	0.9698	7.65	0.9988
0.20	0.0971	2.70	1.5420	5.20	0.9635	7.70	0.9980
0.25	0.5445	2.75	1.8795	5.25	0.9541	7.75	0.9977
0.30	0.7797	2.80	2.0529	5.30	0.9428	7.80	0.9967
0.35	0.8319	2.85	2.0681	5.35	0.9324	7.85	0.9942
0.40	0.7902	2.90	1.9696	5.40	0.9260	7.90	0.9897
0.45	0.7558	2.95	1.8158	5.45	0.9245	7.95	0.9840
0.50	0.7984	3.00	1.6547	5.50	0.9267	8.00	0.9784
0.55	0.9350	3.05	1.5102	5.55	0.9298	8.05	0.9745
0.60	1.1379	3.10	1.3838	5.60	0.9318	8.10	0.9735
0.65	1.3618	3.15	1.2663	5.65	0.9321	8.15	0.9753
0.70	1.5711	3.20	1.1526	5.70	0.9317	8.20	0.9788
0.75	1.7547	3.25	1.0492	5.75	0.9327	8.25	0.9824
0.80	1.9198	3.30	0.9718	5.80	0.9363	8.30	0.9849
0.85	2.0720	3.35	0.9361	5.85	0.9424	8.35	0.9857
0.90	2.1987	3.40	0.9463	5.90	0.9492	8.40	0.9856
0.95	2.2644	3.45	0.9908	5.95	0.9547	8.45	0.9857
1.00	2.2255	3.50	1.0458	6.00	0.9575	8.50	0.9871
1.05	2.0545	3.55	1.0859	6.05	0.9580	8.55	0.9904
1.10	1.7608	3.60	1.0951	6.10	0.9580	8.60	0.9947
1.15	1.3949	3.65	1.0733	6.15	0.9597	8.65	0.9989
1.20	1.0314	3.70	1.0342	6.20	0.9648	8.70	1.0016
1.25	0.7394	3.75	0.9973	6.25	0.9731	8.75	1.0021
1.30	0.5545	3.80	0.9774	6.30	0.9834	8.80	1.0008
1.35	0.4668	3.85	0.9784	6.35	0.9938	8.85	0.9987
1.40	0.4317	3.90	0.9928	6.40	1.0027	8.90	0.9970
1.45	0.3959	3.95	1.0080	6.45	1.0101	8.95	0.9968
1.50	0.3255	4.00	1.0137	6.50	1.0168	9.00	0.9980
1.55	0.2220	4.05	1.0071	6.55	1.0239	9.05	1.0001
1.60	0.1170	4.10	0.9941	6.60	1.0321	9.10	1.0021
1.65	0.0502	4.15	0.9841	6.65	1.0410	9.15	1.0035
1.70	0.0440	4.20	0.9845	6.70	1.0491	9.20	1.0041
1.75	0.0890	4.25	0.9964	6.75	1.0550	9.25	1.0041
1.80	0.1478	4.30	1.0144	6.80	1.0574	9.30	1.0040
1.85	0.1760	4.35	1.0303	6.85	1.0564	9.35	1.0038
1.90	0.1475	4.40	1.0381	6.90	1.0530	9.40	1.0036
1.95	0.0699	4.45	1.0377	6.95	1.0487	9.45	1.0029
2.00	-0.0193	4.50	1.0341	7.00	1.0447	9.50	1.0014
2.05	-0.0737	4.55	1.0346	7.05	1.0417	9.55	0.9992
2.10	-0.0650	4.60	1.0439	7.10	1.0395	9.60	0.9969
2.15	-0.0012	4.65	1.0610	7.15	1.0376	9.65	0.9955
2.20	0.0761	4.70	1.0797	7.20	1.0354	9.70	0.9956
2.25	0.1129	4.75	1.0915	7.25	1.0325	9.75	0.9973
2.30	0.0747	4.80	1.0900	7.30	1.0288	9.80	1.0003
2.35	-0.0303	4.85	1.0741	7.35	1.0244	9.85	1.0034
2.40	-0.1469	4.90	1.0483	7.40	1.0194	9.90	1.0057
2.45	-0.1934	4.95	1.0205	7.45	1.0141	9.95	1.0064

INTENSITIES IN ELECTRON UNITS H_2O 75°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
0.0	0.660E 02	0.100E-01	0.714E 01	0.700E-01	-0.589E 00	0.0	0.0
0.100	0.659E 02	0.100E-01	0.714E 01	0.700E-01	-0.589E 00	-0.589E-01	0.702E-04
0.200	0.656E 02	0.101E-01	0.714E 01	0.700E-01	-0.589E 00	-0.118E 00	0.141E-03
0.300	0.652E 02	0.101E-01	0.714E 01	0.700E-01	-0.588E 00	-0.177E 00	0.213E-03
0.400	0.646E 02	0.102E-01	0.714E 01	0.700E-01	-0.588E 00	-0.235E 00	0.287E-03
0.500	0.638E 02	0.104E-01	0.714E 01	0.700E-01	-0.588E 00	-0.294E 00	0.363E-03
0.533	0.636E 02	0.104E-01	0.720E 01	0.698E-01	-0.587E 00	-0.313E 00	0.388E-03
0.633	0.626E 02	0.106E-01	0.756E 01	0.687E-01	-0.583E 00	-0.369E 00	0.461E-03
0.733	0.616E 02	0.108E-01	0.818E 01	0.667E-01	-0.576E 00	-0.423E 00	0.528E-03
0.833	0.603E 02	0.110E-01	0.907E 01	0.638E-01	-0.566E 00	-0.471E 00	0.587E-03
0.933	0.589E 02	0.113E-01	0.102E 02	0.601E-01	-0.551E 00	-0.515E 00	0.634E-03

H_2O 75°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
1.033	0.575E 02	0.116E-01	0.117E 02	0.555E-01	-0.533E 00	-0.551E 00	0.667E-03
1.133	0.560E 02	0.120E-01	0.133E 02	0.500E-01	-0.511E 00	-0.579E 00	0.679E-03
1.233	0.544E 02	0.124E-01	0.153E 02	0.437E-01	-0.483E 00	-0.596E 00	0.666E-03
1.310	0.531E 02	0.127E-01	0.165E 02	0.471E-01	-0.465E 00	-0.609E 00	0.783E-03
1.387	0.518E 02	0.130E-01	0.195E 02	0.554E-01	-0.421E 00	-0.584E 00	0.100E-02
1.464	0.504E 02	0.134E-01	0.229E 02	0.645E-01	-0.370E 00	-0.542E 00	0.127E-02
1.541	0.491E 02	0.138E-01	0.273E 02	0.764E-01	-0.301E 00	-0.463E 00	0.163E-02
1.618	0.477E 02	0.143E-01	0.320E 02	0.888E-01	-0.224E 00	-0.362E 00	0.205E-02
1.695	0.464E 02	0.147E-01	0.381E 02	0.105E 00	-0.122E 00	-0.207E 00	0.261E-02
1.771	0.450E 02	0.152E-01	0.446E 02	0.122E 00	-0.648E-02	-0.115E-01	0.328E-02
1.848	0.436E 02	0.157E-01	0.507E 02	0.138E 00	0.112E 00	0.207E 00	0.401E-02
1.925	0.422E 02	0.163E-01	0.555E 02	0.151E 00	0.216E 00	0.416E 00	0.472E-02
2.002	0.408E 02	0.169E-01	0.567E 02	0.154E 00	0.269E 00	0.539E 00	0.522E-02
2.078	0.395E 02	0.175E-01	0.564E 02	0.153E 00	0.297E 00	0.617E 00	0.559E-02
2.155	0.382E 02	0.182E-01	0.550E 02	0.150E 00	0.305E 00	0.658E 00	0.587E-02
2.231	0.369E 02	0.189E-01	0.539E 02	0.147E 00	0.322E 00	0.719E 00	0.620E-02
2.308	0.356E 02	0.196E-01	0.503E 02	0.138E 00	0.289E 00	0.668E 00	0.625E-02
2.384	0.343E 02	0.204E-01	0.466E 02	0.128E 00	0.250E 00	0.597E 00	0.625E-02
2.461	0.331E 02	0.213E-01	0.449E 02	0.124E 00	0.252E 00	0.619E 00	0.650E-02
2.537	0.319E 02	0.222E-01	0.423E 02	0.117E 00	0.232E 00	0.589E 00	0.661E-02
2.614	0.307E 02	0.231E-01	0.407E 02	0.113E 00	0.231E 00	0.605E 00	0.684E-02
2.690	0.296E 02	0.241E-01	0.391E 02	0.109E 00	0.229E 00	0.615E 00	0.706E-02
2.766	0.285E 02	0.251E-01	0.368E 02	0.103E 00	0.208E 00	0.575E 00	0.715E-02
2.842	0.274E 02	0.261E-01	0.348E 02	0.980E-01	0.192E 00	0.546E 00	0.728E-02
2.918	0.264E 02	0.273E-01	0.319E 02	0.906E-01	0.150E 00	0.439E 00	0.721E-02
2.994	0.254E 02	0.284E-01	0.292E 02	0.836E-01	0.107E 00	0.322E 00	0.712E-02
3.070	0.244E 02	0.297E-01	0.254E 02	0.742E-01	0.299E-01	0.919E-01	0.677E-02
3.146	0.235E 02	0.310E-01	0.224E 02	0.659E-01	-0.350E-01	-0.110E 00	0.643E-02
3.222	0.226E 02	0.323E-01	0.200E 02	0.601E-01	-0.834E-01	-0.269E 00	0.626E-02
3.298	0.217E 02	0.338E-01	0.176E 02	0.537E-01	-0.138E 00	-0.454E 00	0.598E-02
3.374	0.209E 02	0.353E-01	0.161E 02	0.493E-01	-0.168E 00	-0.568E 00	0.587E-02
3.450	0.200E 02	0.369E-01	0.145E 02	0.455E-01	-0.206E 00	-0.710E 00	0.578E-02
3.525	0.193E 02	0.385E-01	0.141E 02	0.386E-01	-0.199E 00	-0.701E 00	0.523E-02
3.676	0.178E 02	0.420E-01	0.131E 02	0.363E-01	-0.197E 00	-0.724E 00	0.560E-02
3.827	0.164E 02	0.458E-01	0.127E 02	0.354E-01	-0.170E 00	-0.649E 00	0.621E-02
3.978	0.152E 02	0.499E-01	0.126E 02	0.352E-01	-0.127E 00	-0.507E 00	0.698E-02
4.128	0.141E 02	0.543E-01	0.125E 02	0.347E-01	-0.869E-01	-0.359E 00	0.778E-02
4.278	0.130E 02	0.591E-01	0.124E 02	0.345E-01	-0.365E-01	-0.156E 00	0.872E-02
4.427	0.121E 02	0.641E-01	0.121E 02	0.336E-01	-0.400E-02	-0.177E-01	0.954E-02
4.576	0.113E 02	0.694E-01	0.117E 02	0.327E-01	0.287E-01	0.131E 00	0.104E-01
4.725	0.105E 02	0.753E-01	0.111E 02	0.313E-01	0.476E-01	0.225E 00	0.111E-01
4.874	0.975E 01	0.814E-01	0.103E 02	0.293E-01	0.407E-01	0.198E 00	0.116E-01
5.022	0.911E 01	0.877E-01	0.940E 01	0.273E-01	0.259E-01	0.130E 00	0.120E-01
5.170	0.851E 01	0.946E-01	0.867E 01	0.256E-01	0.157E-01	0.811E-01	0.125E-01
5.317	0.797E 01	0.102E 00	0.789E 01	0.237E-01	-0.803E-02	-0.427E-01	0.128E-01
5.464	0.750E 01	0.109E 00	0.713E 01	0.219E-01	-0.404E-01	-0.221E 00	0.130E-01
5.610	0.705E 01	0.117E 00	0.655E 01	0.205E-01	-0.589E-01	-0.330E 00	0.134E-01
5.757	0.665E 01	0.125E 00	0.607E 01	0.193E-01	-0.723E-01	-0.416E 00	0.138E-01
5.902	0.628E 01	0.133E 00	0.570E 01	0.183E-01	-0.777E-01	-0.458E 00	0.143E-01
6.047	0.595E 01	0.141E 00	0.546E 01	0.176E-01	-0.700E-01	-0.423E 00	0.150E-01
6.192	0.564E 01	0.150E 00	0.530E 01	0.170E-01	-0.510E-01	-0.316E 00	0.158E-01
6.337	0.536E 01	0.158E 00	0.518E 01	0.166E-01	-0.294E-01	-0.186E 00	0.166E-01
6.480	0.511E 01	0.167E 00	0.508E 01	0.162E-01	-0.589E-02	-0.381E-01	0.175E-01
6.624	0.488E 01	0.176E 00	0.496E 01	0.157E-01	0.145E-01	0.962E-01	0.183E-01
6.766	0.466E 01	0.185E 00	0.491E 01	0.154E-01	0.459E-01	0.311E 00	0.193E-01
6.909	0.447E 01	0.194E 00	0.477E 01	0.148E-01	0.575E-01	0.397E 00	0.199E-01
7.051	0.430E 01	0.203E 00	0.460E 01	0.143E-01	0.616E-01	0.434E 00	0.205E-01
7.192	0.413E 01	0.213E 00	0.440E 01	0.137E-01	0.576E-01	0.414E 00	0.209E-01
7.332	0.398E 01	0.222E 00	0.420E 01	0.826E-02	0.475E-01	0.349E 00	0.134E-01
7.473	0.384E 01	0.231E 00	0.399E 01	0.786E-02	0.328E-01	0.245E 00	0.136E-01
7.612	0.372E 01	0.240E 00	0.377E 01	0.745E-02	0.135E-01	0.103E 00	0.136E-01
7.751	0.360E 01	0.249E 00	0.361E 01	0.710E-02	0.309E-02	0.239E-01	0.137E-01
7.890	0.349E 01	0.258E 00	0.345E 01	0.677E-02	-0.973E-02	-0.768E-01	0.138E-01
8.027	0.339E 01	0.266E 00	0.331E 01	0.645E-02	-0.224E-01	-0.179E 00	0.138E-01
8.164	0.329E 01	0.275E 00	0.322E 01	0.622E-02	-0.215E-01	-0.176E 00	0.140E-01
8.301	0.321E 01	0.284E 00	0.311E 01	0.598E-02	-0.270E-01	-0.224E 00	0.141E-01
8.437	0.313E 01	0.292E 00	0.305E 01	0.580E-02	-0.209E-01	-0.176E 00	0.143E-01
8.572	0.305E 01	0.300E 00	0.301E 01	0.565E-02	-0.111E-01	-0.952E-01	0.145E-01
8.707	0.298E 01	0.309E 00	0.297E 01	0.550E-02	-0.299E-02	-0.260E-01	0.148E-01
8.841	0.291E 01	0.317E 00	0.294E 01	0.539E-02	0.979E-02	0.865E-01	0.151E-01
8.974	0.285E 01	0.324E 00	0.290E 01	0.524E-02	0.148E-01	0.133E 00	0.152E-01
9.107	0.279E 01	0.332E 00	0.286E 01	0.513E-02	0.235E-01	0.214E 00	0.155E-01
9.239	0.274E 01	0.340E 00	0.282E 01	0.500E-02	0.275E-01	0.254E 00	0.157E-01
9.370	0.269E 01	0.347E 00	0.276E 01	0.486E-02	0.261E-01	0.245E 00	0.158E-01
9.500	0.264E 01	0.355E 00	0.271E 01	0.473E-02	0.238E-01	0.226E 00	0.159E-01
9.630	0.259E 01	0.362E 00	0.265E 01	0.460E-02	0.203E-01	0.195E 00	0.160E-01

H_2O 75°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
9.759	0.255E 01	0.369E 00	0.258E 01	0.446E-02	0.114E-01	0.112E 00	0.160E-01
9.887	0.251E 01	0.376E 00	0.251E 01	0.431E-02	0.154E-02	0.152E-01	0.160E-01
10.015	0.247E 01	0.382E 00	0.245E 01	0.419E-02	-0.478E-02	-0.479E-01	0.161E-01
10.142	0.243E 01	0.389E 00	0.240E 01	0.407E-02	-0.112E-01	-0.114E 00	0.161E-01
10.268	0.239E 01	0.396E 00	0.234E 01	0.395E-02	-0.186E-01	-0.191E 00	0.161E-01
10.393	0.236E 01	0.403E 00	0.232E 01	0.387E-02	-0.168E-01	-0.175E 00	0.162E-01
10.517	0.233E 01	0.409E 00	0.228E 01	0.377E-02	-0.205E-01	-0.216E 00	0.162E-01
10.641	0.229E 01	0.416E 00	0.225E 01	0.370E-02	-0.185E-01	-0.197E 00	0.164E-01
10.764	0.226E 01	0.422E 00	0.223E 01	0.365E-02	-0.140E-01	-0.151E 00	0.166E-01
10.886	0.224E 01	0.429E 00	0.221E 01	0.359E-02	-0.107E-01	-0.116E 00	0.167E-01
11.007	0.221E 01	0.435E 00	0.220E 01	0.353E-02	-0.573E-02	-0.631E-01	0.169E-01
11.127	0.218E 01	0.442E 00	0.218E 01	0.349E-02	-0.483E-03	-0.537E-02	0.172E-01
11.247	0.215E 01	0.448E 00	0.216E 01	0.344E-02	0.335E-02	0.376E-01	0.173E-01
11.366	0.213E 01	0.454E 00	0.213E 01	0.337E-02	0.181E-02	0.206E-01	0.174E-01
11.483	0.210E 01	0.460E 00	0.212E 01	0.332E-02	0.642E-02	0.737E-01	0.175E-01
11.600	0.208E 01	0.466E 00	0.209E 01	0.326E-02	0.610E-02	0.707E-01	0.176E-01
11.716	0.206E 01	0.472E 00	0.206E 01	0.320E-02	0.374E-02	0.439E-01	0.177E-01
11.831	0.203E 01	0.477E 00	0.205E 01	0.315E-02	0.746E-02	0.882E-01	0.178E-01
11.946	0.201E 01	0.483E 00	0.202E 01	0.309E-02	0.531E-02	0.634E-01	0.178E-01
12.059	0.199E 01	0.488E 00	0.200E 01	0.304E-02	0.363E-02	0.438E-01	0.179E-01
12.171	0.197E 01	0.494E 00	0.197E 01	0.299E-02	0.158E-03	0.193E-02	0.180E-01
12.283	0.195E 01	0.499E 00	0.194E 01	0.295E-02	-0.187E-02	-0.230E-01	0.181E-01
12.393	0.193E 01	0.505E 00	0.192E 01	0.290E-02	-0.458E-02	-0.568E-01	0.181E-01
12.503	0.191E 01	0.510E 00	0.190E 01	0.287E-02	-0.309E-02	-0.386E-01	0.183E-01
12.611	0.189E 01	0.516E 00	0.188E 01	0.283E-02	-0.513E-02	-0.647E-01	0.184E-01
12.719	0.187E 01	0.522E 00	0.186E 01	0.279E-02	-0.478E-02	-0.608E-01	0.185E-01
12.826	0.185E 01	0.528E 00	0.184E 01	0.276E-02	-0.464E-02	-0.595E-01	0.187E-01
12.932	0.183E 01	0.534E 00	0.182E 01	0.272E-02	-0.569E-02	-0.736E-01	0.188E-01
13.036	0.181E 01	0.540E 00	0.180E 01	0.269E-02	-0.670E-02	-0.873E-01	0.189E-01
13.140	0.179E 01	0.546E 00	0.179E 01	0.267E-02	-0.471E-02	-0.618E-01	0.192E-01
13.243	0.178E 01	0.552E 00	0.177E 01	0.265E-02	-0.616E-02	-0.815E-01	0.194E-01
13.345	0.176E 01	0.558E 00	0.175E 01	0.264E-02	-0.240E-02	-0.321E-01	0.196E-01
13.445	0.174E 01	0.565E 00	0.174E 01	0.261E-02	-0.227E-02	-0.306E-01	0.199E-01
13.545	0.172E 01	0.571E 00	0.172E 01	0.259E-02	-0.192E-02	-0.261E-01	0.201E-01
13.644	0.170E 01	0.577E 00	0.170E 01	0.257E-02	-0.137E-02	-0.186E-01	0.202E-01
13.741	0.169E 01	0.583E 00	0.169E 01	0.256E-02	0.156E-02	0.214E-01	0.205E-01
13.838	0.167E 01	0.589E 00	0.167E 01	0.253E-02	0.169E-02	0.234E-01	0.206E-01
13.933	0.165E 01	0.595E 00	0.166E 01	0.251E-02	0.288E-02	0.401E-01	0.208E-01
14.028	0.164E 01	0.600E 00	0.164E 01	0.250E-02	0.457E-02	0.641E-01	0.210E-01
14.121	0.162E 01	0.606E 00	0.163E 01	0.247E-02	0.398E-02	0.562E-01	0.212E-01
14.214	0.160E 01	0.612E 00	0.161E 01	0.246E-02	0.548E-02	0.779E-01	0.214E-01
14.305	0.158E 01	0.623E 00	0.158E 01	0.241E-02	0.285E-02	0.411E-01	0.216E-01
14.572	0.155E 01	0.634E 00	0.156E 01	0.238E-02	0.501E-02	0.730E-01	0.220E-01
14.744	0.152E 01	0.645E 00	0.153E 01	0.234E-02	0.262E-02	0.386E-01	0.223E-01
14.913	0.150E 01	0.656E 00	0.150E 01	0.231E-02	0.102E-02	0.152E-01	0.226E-01
15.076	0.148E 01	0.668E 00	0.148E 01	0.228E-02	-0.651E-03	-0.982E-02	0.229E-01
15.235	0.145E 01	0.679E 00	0.145E 01	0.225E-02	-0.569E-02	-0.866E-01	0.233E-01
15.389	0.143E 01	0.691E 00	0.142E 01	0.223E-02	-0.470E-02	-0.724E-01	0.237E-01
15.539	0.140E 01	0.702E 00	0.139E 01	0.220E-02	-0.678E-02	-0.105E 00	0.241E-01
15.684	0.138E 01	0.713E 00	0.137E 01	0.217E-02	-0.962E-02	-0.151E 00	0.243E-01
15.824	0.136E 01	0.723E 00	0.136E 01	0.216E-02	-0.452E-02	-0.715E-01	0.247E-01
15.959	0.135E 01	0.732E 00	0.134E 01	0.214E-02	-0.384E-02	-0.612E-01	0.250E-01

RADIAL DISTRIBUTION FUNCTIONS TO 10 A

H_2O 75°C

R	G(R)	R	G(R)	R	G(R)	R	G(R)
0.0	0.0	2.50	0.1053	5.00	0.9929	7.50	1.0163
0.05	-2.0350	2.55	0.3081	5.05	0.9938	7.55	1.0106
0.10	-1.6081	2.60	0.6231	5.10	0.9944	7.60	1.0030
0.15	-1.0504	2.65	0.9963	5.15	0.9912	7.65	0.9951
0.20	-0.5278	2.70	1.3567	5.20	0.9831	7.70	0.9889
0.25	-0.1718	2.75	1.6412	5.25	0.9724	7.75	0.9855
0.30	-0.0346	2.80	1.8133	5.30	0.9629	7.80	0.9849
0.35	-0.0792	2.85	1.8698	5.35	0.9579	7.85	0.9861
0.40	-0.2053	2.90	1.8337	5.40	0.9581	7.90	0.9876
0.45	-0.2989	2.95	1.7399	5.45	0.9614	7.95	0.9884
0.50	-0.2779	3.00	1.6203	5.50	0.9643	8.00	0.9880
0.55	-0.1182	3.05	1.4957	5.55	0.9636	8.05	0.9870
0.60	0.1503	3.10	1.3757	5.60	0.9588	8.10	0.9862
0.65	0.4693	3.15	1.2644	5.65	0.9520	8.15	0.9861
0.70	0.7830	3.20	1.1666	5.70	0.9468	8.20	0.9867
0.75	1.0592	3.25	1.0902	5.75	0.9461	8.25	0.9876
0.80	1.2908	3.30	1.0433	5.80	0.9504	8.30	0.9884

H_2O 75°C

R	G(R)	R	G(R)	R	G(R)	R	G(R)
0.85	1.4823	3.35	1.0292	5.85	0.9578	8.35	0.9889
0.90	1.6330	3.40	1.0422	5.90	0.9649	8.40	0.9896
0.95	1.7271	3.45	1.0683	5.95	0.9687	8.45	0.9908
1.00	1.7387	3.50	1.0899	6.00	0.9687	8.50	0.9929
1.05	1.6484	3.55	1.0938	6.05	0.9667	8.55	0.9955
1.10	1.4594	3.60	1.0764	6.10	0.9657	8.60	0.9977
1.15	1.2043	3.65	1.0449	6.15	0.9686	8.65	0.9985
1.20	0.9361	3.70	1.0124	6.20	0.9763	8.70	0.9976
1.25	0.7081	3.75	0.9913	6.25	0.9874	8.75	0.9956
1.30	0.5528	3.80	0.9872	6.30	0.9990	8.80	0.9936
1.35	0.4701	3.85	0.9966	6.35	1.0083	8.85	0.9929
1.40	0.4321	3.90	1.0102	6.40	1.0138	8.90	0.9943
1.45	0.4010	3.95	1.0180	6.45	1.0160	8.95	0.9975
1.50	0.3497	4.00	1.0151	6.50	1.0169	9.00	1.0012
1.55	0.2747	4.05	1.0032	6.55	1.0183	9.05	1.0039
1.60	0.1955	4.10	0.9890	6.60	1.0213	9.10	1.0046
1.65	0.1401	4.15	0.9798	6.65	1.0253	9.15	1.0031
1.70	0.1273	4.20	0.9794	6.70	1.0290	9.20	1.0007
1.75	0.1547	4.25	0.9862	6.75	1.0313	9.25	0.9989
1.80	0.1998	4.30	0.9951	6.80	1.0316	9.30	0.9988
1.85	0.2331	4.35	1.0008	6.85	1.0309	9.35	1.0007
1.90	0.2351	4.40	1.0010	6.90	1.0301	9.40	1.0036
1.95	0.2074	4.45	0.9978	6.95	1.0304	9.45	1.0061
2.00	0.1713	4.50	0.9959	7.00	1.0316	9.50	1.0070
2.05	0.1546	4.55	0.9994	7.05	1.0329	9.55	1.0059
2.10	0.1737	4.60	1.0090	7.10	1.0331	9.60	1.0034
2.15	0.2218	4.65	1.0215	7.15	1.0316	9.65	1.0008
2.20	0.2706	4.70	1.0314	7.20	1.0286	9.70	0.9993
2.25	0.2852	4.75	1.0340	7.25	1.0252	9.75	0.9994
2.30	0.2448	4.80	1.0281	7.30	1.0226	9.80	1.0007
2.35	0.1588	4.85	1.0164	7.35	1.0213	9.85	1.0021
2.40	0.0685	4.90	1.0041	7.40	1.0207	9.90	1.0027
2.45	0.0231	4.95	0.9957	7.45	1.0195	9.95	1.0020

INTENSITIES IN ELECTRON UNITS H_2O 100°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
0.0	0.660E 02	0.100E-01	0.807E 01	0.800E-01	-0.579E 00	0.0	0.0
0.100	0.659E 02	0.100E-01	0.807E 01	0.800E-01	-0.579E 00	-0.579E-01	0.802E-04
0.200	0.656E 02	0.101E-01	0.807E 01	0.800E-01	-0.579E 00	-0.116E 00	0.161E-03
0.300	0.652E 02	0.101E-01	0.807E 01	0.800E-01	-0.579E 00	-0.174E 00	0.243E-03
0.400	0.646E 02	0.102E-01	0.807E 01	0.800E-01	-0.579E 00	-0.232E 00	0.328E-03
0.500	0.638E 02	0.104E-01	0.807E 01	0.800E-01	-0.578E 00	-0.289E 00	0.415E-03
0.533	0.636E 02	0.104E-01	0.812E 01	0.797E-01	-0.578E 00	-0.308E 00	0.443E-03
0.633	0.626E 02	0.106E-01	0.840E 01	0.780E-01	-0.574E 00	-0.364E 00	0.524E-03
0.733	0.616E 02	0.108E-01	0.889E 01	0.751E-01	-0.568E 00	-0.417E 00	0.595E-03
0.833	0.603E 02	0.110E-01	0.960E 01	0.709E-01	-0.560E 00	-0.467E 00	0.652E-03
0.933	0.589E 02	0.113E-01	0.105E 02	0.655E-01	-0.548E 00	-0.512E 00	0.692E-03
1.033	0.575E 02	0.116E-01	0.116E 02	0.587E-01	-0.533E 00	-0.551E 00	0.707E-03
1.133	0.560E 02	0.120E-01	0.130E 02	0.508E-01	-0.515E 00	-0.584E 00	0.689E-03
1.233	0.544E 02	0.124E-01	0.145E 02	0.415E-01	-0.493E 00	-0.608E 00	0.633E-03
1.310	0.531E 02	0.127E-01	0.160E 02	0.458E-01	-0.471E 00	-0.617E 00	0.761E-03
1.387	0.518E 02	0.130E-01	0.186E 02	0.527E-01	-0.433E 00	-0.601E 00	0.954E-03
1.464	0.504E 02	0.134E-01	0.213E 02	0.602E-01	-0.391E 00	-0.572E 00	0.118E-02
1.541	0.491E 02	0.138E-01	0.255E 02	0.713E-01	-0.326E 00	-0.503E 00	0.152E-02
1.618	0.477E 02	0.143E-01	0.289E 02	0.803E-01	-0.269E 00	-0.436E 00	0.185E-02
1.695	0.464E 02	0.147E-01	0.348E 02	0.960E-01	-0.170E 00	-0.288E 00	0.239E-02
1.771	0.450E 02	0.152E-01	0.400E 02	0.109E 00	-0.769E-01	-0.136E 00	0.295E-02
1.848	0.436E 02	0.157E-01	0.455E 02	0.124E 00	0.291E-01	0.538E-01	0.361E-02
1.925	0.422E 02	0.163E-01	0.483E 02	0.132E 00	0.985E-01	0.190E 00	0.413E-02
2.002	0.408E 02	0.169E-01	0.511E 02	0.139E 00	0.174E 00	0.349E 00	0.471E-02
2.078	0.395E 02	0.175E-01	0.518E 02	0.141E 00	0.215E 00	0.447E 00	0.514E-02
2.155	0.382E 02	0.182E-01	0.509E 02	0.139E 00	0.231E 00	0.497E 00	0.545E-02
2.231	0.369E 02	0.189E-01	0.497E 02	0.136E 00	0.242E 00	0.540E 00	0.574E-02
2.308	0.356E 02	0.196E-01	0.477E 02	0.131E 00	0.238E 00	0.550E 00	0.595E-02
2.384	0.343E 02	0.204E-01	0.440E 02	0.122E 00	0.197E 00	0.470E 00	0.593E-02
2.461	0.331E 02	0.213E-01	0.416E 02	0.116E 00	0.181E 00	0.444E 00	0.606E-02
2.537	0.319E 02	0.222E-01	0.392E 02	0.110E 00	0.163E 00	0.415E 00	0.618E-02
2.614	0.307E 02	0.231E-01	0.385E 02	0.108E 00	0.179E 00	0.468E 00	0.652E-02
2.690	0.296E 02	0.241E-01	0.365E 02	0.103E 00	0.167E 00	0.450E 00	0.668E-02
2.766	0.285E 02	0.251E-01	0.349E 02	0.992E-01	0.160E 00	0.443E 00	0.688E-02
2.842	0.274E 02	0.261E-01	0.330E 02	0.944E-01	0.145E 00	0.412E 00	0.702E-02

						H_2O	100°C
S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
2.918	0.264E 02	0.273E-01	0.310E 02	0.896E-01	0.126E 00	0.367E 00	0.713E-02
2.994	0.254E 02	0.284E-01	0.296E 02	0.835E-01	0.910E-01	0.272E 00	0.711E-02
3.070	0.244E 02	0.297E-01	0.253E 02	0.751E-01	0.246E-01	0.754E-01	0.684E-02
3.146	0.235E 02	0.310E-01	0.225E 02	0.681E-01	-0.305E-01	-0.959E-01	0.664E-02
3.222	0.226E 02	0.323E-01	0.202E 02	0.621E-01	-0.779E-01	-0.251E 00	0.647E-02
3.298	0.217E 02	0.339E-01	0.181E 02	0.571E-01	-0.120E 00	-0.397E 00	0.637E-02
3.374	0.209E 02	0.353E-01	0.168E 02	0.539E-01	-0.144E 00	-0.485E 00	0.642E-02
3.450	0.200E 02	0.369E-01	0.154E 02	0.505E-01	-0.170E 00	-0.585E 00	0.641E-02
3.525	0.193E 02	0.385E-01	0.144E 02	0.476E-01	-0.185E 00	-0.653E 00	0.564E-02
3.676	0.178E 02	0.420E-01	0.135E 02	0.397E-01	-0.180E 00	-0.661E 00	0.613E-02
3.827	0.164E 02	0.458E-01	0.129E 02	0.386E-01	-0.162E 00	-0.622E 00	0.676E-02
3.978	0.152E 02	0.499E-01	0.129E 02	0.387E-01	-0.117E 00	-0.464E 00	0.768E-02
4.128	0.141E 02	0.543E-01	0.128E 02	0.388E-01	-0.691E-01	-0.285E 00	0.869E-02
4.278	0.130E 02	0.591E-01	0.126E 02	0.385E-01	-0.276E-01	-0.118E 00	0.971E-02
4.427	0.121E 02	0.641E-01	0.123E 02	0.379E-01	0.935E-02	0.414E-01	0.108E-01
4.576	0.113E 02	0.694E-01	0.117E 02	0.368E-01	0.289E-01	0.132E 00	0.117E-01
4.725	0.105E 02	0.753E-01	0.109E 02	0.351E-01	0.329E-01	0.156E 00	0.125E-01
4.874	0.975E 01	0.814E-01	0.101E 02	0.335E-01	0.322E-01	0.157E 00	0.133E-01
5.022	0.911E 01	0.877E-01	0.932E 01	0.317E-01	0.191E-01	0.957E-01	0.140E-01
5.170	0.851E 01	0.946E-01	0.862E 01	0.300E-01	0.104E-01	0.538E-01	0.147E-01
5.317	0.797E 01	0.102E 00	0.782E 01	0.282E-01	-0.153E-01	-0.815E-01	0.153E-01
5.464	0.750E 01	0.109E 00	0.708E 01	0.265E-01	-0.453E-01	-0.248E 00	0.158E-01
5.610	0.705E 01	0.117E 00	0.664E 01	0.255E-01	-0.481E-01	-0.270E 00	0.167E-01
5.757	0.665E 01	0.125E 00	0.611E 01	0.243E-01	-0.664E-01	-0.382E 00	0.174E-01
5.902	0.628E 01	0.133E 00	0.575E 01	0.234E-01	-0.705E-01	-0.416E 00	0.183E-01
6.047	0.595E 01	0.141E 00	0.564E 01	0.231E-01	-0.434E-01	-0.262E 00	0.197E-01
6.192	0.564E 01	0.150E 00	0.547E 01	0.224E-01	-0.264E-01	-0.163E 00	0.208E-01
6.337	0.536E 01	0.158E 00	0.545E 01	0.221E-01	0.145E-01	0.919E-01	0.222E-01
6.480	0.511E 01	0.167E 00	0.512E 01	0.211E-01	0.206E-02	0.134E-01	0.229E-01
6.624	0.488E 01	0.176E 00	0.491E 01	0.203E-01	0.642E-02	0.425E-01	0.237E-01
6.766	0.466E 01	0.185E 00	0.481E 01	0.197E-01	0.273E-01	0.189E 00	0.247E-01
6.909	0.447E 01	0.194E 00	0.462E 01	0.188E-01	0.286E-01	0.197E 00	0.252E-01
7.051	0.430E 01	0.203E 00	0.452E 01	0.183E-01	0.450E-01	0.317E 00	0.262E-01
7.192	0.413E 01	0.213E 00	0.435E 01	0.176E-01	0.458E-01	0.330E 00	0.270E-01
7.332	0.398E 01	0.222E 00	0.415E 01	0.167E-01	0.368E-01	0.270E 00	0.274E-01
7.473	0.384E 01	0.231E 00	0.396E 01	0.162E-01	0.256E-01	0.192E 00	0.276E-01
7.612	0.372E 01	0.240E 00	0.379E 01	0.977E-02	0.185E-01	0.141E 00	0.178E-01
7.751	0.360E 01	0.249E 00	0.364E 01	0.933E-02	0.116E-01	0.898E-01	0.180E-01
7.890	0.349E 01	0.258E 00	0.348E 01	0.886E-02	-0.342E-02	-0.270E-01	0.180E-01
8.027	0.339E 01	0.266E 00	0.337E 01	0.849E-02	-0.615E-02	-0.494E-01	0.181E-01
8.164	0.329E 01	0.275E 00	0.326E 01	0.815E-02	-0.109E-01	-0.889E-01	0.183E-01
8.301	0.321E 01	0.284E 00	0.318E 01	0.786E-02	-0.829E-02	-0.688E-01	0.185E-01
8.437	0.313E 01	0.292E 00	0.309E 01	0.757E-02	-0.940E-02	-0.793E-01	0.186E-01
8.572	0.305E 01	0.300E 00	0.303E 01	0.731E-02	-0.677E-02	-0.581E-01	0.188E-01
8.707	0.298E 01	0.309E 00	0.297E 01	0.708E-02	-0.328E-02	-0.285E-01	0.190E-01
8.841	0.291E 01	0.317E 00	0.292E 01	0.687E-02	0.115E-02	0.101E-01	0.192E-01
8.974	0.285E 01	0.324E 00	0.288E 01	0.667E-02	0.981E-02	0.881E-01	0.194E-01
9.107	0.279E 01	0.332E 00	0.283E 01	0.645E-02	0.121E-01	0.110E 00	0.195E-01
9.239	0.274E 01	0.340E 00	0.279E 01	0.625E-02	0.189E-01	0.175E 00	0.196E-01
9.370	0.269E 01	0.347E 00	0.273E 01	0.601E-02	0.160E-01	0.150E 00	0.196E-01
9.500	0.264E 01	0.355E 00	0.268E 01	0.578E-02	0.136E-01	0.129E 00	0.195E-01
9.630	0.259E 01	0.362E 00	0.264E 01	0.562E-02	0.154E-01	0.149E 00	0.196E-01
9.759	0.255E 01	0.369E 00	0.258E 01	0.543E-02	0.999E-02	0.975E-01	0.196E-01
9.887	0.251E 01	0.376E 00	0.251E 01	0.523E-02	0.134E-02	0.133E-01	0.195E-01
10.015	0.247E 01	0.382E 00	0.246E 01	0.507E-02	-0.117E-02	-0.117E-01	0.194E-01
10.142	0.243E 01	0.389E 00	0.241E 01	0.491E-02	-0.773E-02	-0.784E-01	0.194E-01
10.269	0.239E 01	0.395E 00	0.237E 01	0.477E-02	-0.857E-02	-0.880E-01	0.194E-01
10.393	0.236E 01	0.403E 00	0.233E 01	0.463E-02	-0.110E-01	-0.115E 00	0.194E-01
10.517	0.233E 01	0.409E 00	0.230E 01	0.450E-02	-0.112E-01	-0.119E 00	0.194E-01
10.641	0.229E 01	0.416E 00	0.225E 01	0.438E-02	-0.170E-01	-0.180E 00	0.194E-01
10.764	0.226E 01	0.422E 00	0.224E 01	0.430E-02	-0.109E-01	-0.118E 00	0.195E-01
10.886	0.224E 01	0.429E 00	0.222E 01	0.421E-02	-0.801E-02	-0.872E-01	0.197E-01
11.007	0.221E 01	0.435E 00	0.219E 01	0.413E-02	-0.766E-02	-0.844E-01	0.198E-01
11.127	0.218E 01	0.442E 00	0.217E 01	0.405E-02	-0.414E-02	-0.460E-01	0.199E-01
11.247	0.215E 01	0.448E 00	0.215E 01	0.397E-02	-0.112E-02	-0.126E-01	0.200E-01
11.366	0.213E 01	0.454E 00	0.213E 01	0.390E-02	-0.339E-03	-0.386E-02	0.201E-01
11.483	0.210E 01	0.460E 00	0.210E 01	0.383E-02	0.277E-03	0.318E-02	0.202E-01
11.600	0.208E 01	0.466E 00	0.209E 01	0.378E-02	0.611E-02	0.709E-01	0.204E-01
11.716	0.206E 01	0.472E 00	0.206E 01	0.370E-02	0.328E-02	0.385E-01	0.205E-01
11.831	0.203E 01	0.477E 00	0.205E 01	0.365E-02	0.743E-02	0.879E-01	0.206E-01
11.946	0.201E 01	0.483E 00	0.202E 01	0.358E-02	0.515E-02	0.615E-01	0.207E-01
12.059	0.199E 01	0.488E 00	0.199E 01	0.352E-02	0.290E-02	0.350E-01	0.207E-01
12.171	0.197E 01	0.494E 00	0.198E 01	0.347E-02	0.398E-02	0.484E-01	0.209E-01
12.283	0.195E 01	0.499E 00	0.195E 01	0.341E-02	-0.112E-02	-0.138E-01	0.209E-01
12.393	0.193E 01	0.505E 00	0.193E 01	0.336E-02	0.221E-03	0.274E-02	0.210E-01
12.503	0.191E 01	0.510E 00	0.191E 01	0.331E-02	-0.557E-03	-0.696E-02	0.211E-01

H_2O 100°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
12.611	0.189E 01	0.514E 00	0.188E 01	0.227E-02	-0.255E-02	-0.322E-01	0.213E-01
12.719	0.187E 01	0.522E 00	0.186E 01	0.322E-02	-0.695E-02	-0.884E-01	0.213E-01
12.826	0.185E 01	0.529E 00	0.184E 01	0.319E-02	-0.370E-02	-0.474E-01	0.216E-01
12.932	0.183E 01	0.534E 00	0.182E 01	0.314E-02	-0.538E-02	-0.696E-01	0.217E-01
13.036	0.181E 01	0.540E 00	0.181E 01	0.311E-02	-0.328E-02	-0.427E-01	0.219E-01
13.140	0.179E 01	0.546E 00	0.179E 01	0.309E-02	-0.280E-02	-0.368E-01	0.221E-01
13.243	0.178E 01	0.552E 00	0.177E 01	0.305E-02	-0.547E-02	-0.724E-01	0.223E-01
13.345	0.176E 01	0.558E 00	0.175E 01	0.302E-02	-0.401E-02	-0.536E-01	0.225E-01
13.445	0.174E 01	0.565E 00	0.173E 01	0.300E-02	-0.391E-02	-0.526E-01	0.227E-01
13.545	0.172E 01	0.571E 00	0.172E 01	0.298E-02	-0.664E-04	-0.900E-03	0.230E-01
13.644	0.170E 01	0.577E 00	0.170E 01	0.295E-02	-0.150E-02	-0.205E-01	0.232E-01
13.741	0.169E 01	0.583E 00	0.169E 01	0.293E-02	0.509E-03	0.700E-02	0.235E-01
13.838	0.167E 01	0.589E 00	0.167E 01	0.291E-02	0.321E-02	0.444E-01	0.237E-01
13.933	0.165E 01	0.595E 00	0.166E 01	0.289E-02	0.347E-02	0.483E-01	0.239E-01
14.028	0.164E 01	0.600E 00	0.164E 01	0.286E-02	0.405E-02	0.568E-01	0.241E-01
14.214	0.160E 01	0.612E 00	0.161E 01	0.282E-02	0.382E-02	0.543E-01	0.245E-01
14.395	0.159E 01	0.623E 00	0.158E 01	0.278E-02	0.304E-02	0.438E-01	0.249E-01
14.572	0.155E 01	0.634E 00	0.156E 01	0.274E-02	0.397E-02	0.579E-01	0.253E-01
14.744	0.152E 01	0.645E 00	0.152E 01	0.269E-02	-0.298E-02	-0.440E-01	0.256E-01
14.913	0.150E 01	0.656E 00	0.150E 01	0.267E-02	0.163E-02	0.250E-01	0.261E-01
15.076	0.148E 01	0.668E 00	0.147E 01	0.263E-02	-0.469E-02	-0.707E-01	0.265E-01
15.235	0.145E 01	0.679E 00	0.144E 01	0.259E-02	-0.903E-02	-0.138E 00	0.268E-01
15.389	0.143E 01	0.691E 00	0.142E 01	0.257E-02	-0.535E-02	-0.823E-01	0.273E-01
15.539	0.140E 01	0.702E 00	0.140E 01	0.254E-02	-0.300E-02	-0.467E-01	0.277E-01
15.684	0.138E 01	0.713E 00	0.138E 01	0.252E-02	-0.476E-04	-0.746E-03	0.282E-01
15.824	0.136E 01	0.723E 00	0.136E 01	0.249E-02	-0.274E-02	-0.433E-01	0.285E-01
15.959	0.135E 01	0.732E 00	0.134E 01	0.247E-02	-0.993E-03	-0.158E-01	0.289E-01

RADIAL DISTRIBUTION FUNCTIONS TO 10 A

H_2O 100°C

R	G(R)	R	G(R)	R	G(R)	R	G(R)
0.0	0.0	2.60	0.3242	5.00	0.9909	7.50	1.0004
0.05	-1.7715	2.65	0.4047	5.05	0.9868	7.55	0.9948
0.10	-1.4501	2.60	0.7357	5.10	0.9865	7.60	0.9919
0.15	-1.0337	2.65	1.0200	5.15	0.9889	7.65	0.9906
0.20	-0.6519	2.70	1.2982	5.20	0.9916	7.70	0.9894
0.25	-0.4077	2.75	1.5173	5.25	0.9918	7.75	0.9873
0.30	-0.3422	2.80	1.6466	5.30	0.9879	7.80	0.9843
0.35	-0.4251	2.85	1.6817	5.35	0.9804	7.85	0.9814
0.40	-0.5726	2.90	1.6434	5.40	0.9710	7.90	0.9802
0.45	-0.6867	2.95	1.5655	5.45	0.9619	7.95	0.9818
0.50	-0.6924	3.00	1.4810	5.50	0.9545	8.00	0.9859
0.55	-0.5620	3.05	1.4103	5.55	0.9491	8.05	0.9911
0.60	-0.3152	3.10	1.3579	5.60	0.9450	8.10	0.9957
0.65	-0.0019	3.15	1.3161	5.65	0.9413	8.15	0.9981
0.70	0.3238	3.20	1.2739	5.70	0.9381	8.20	0.9976
0.75	0.6230	3.25	1.2245	5.75	0.9363	8.25	0.9952
0.80	0.8793	3.30	1.1697	5.80	0.9375	8.30	0.9922
0.85	1.0910	3.35	1.1173	5.85	0.9432	8.35	0.9903
0.90	1.2585	3.40	1.0761	5.90	0.9535	8.40	0.9901
0.95	1.3742	3.45	1.0502	5.95	0.9669	8.45	0.9914
1.00	1.4221	3.50	1.0369	6.00	0.9805	8.50	0.9929
1.05	1.3866	3.55	1.0346	6.05	0.9892	8.55	0.9935
1.10	1.2649	3.60	1.0368	6.10	1.0022	8.60	0.9929
1.15	1.0752	3.65	0.9976	6.15	1.0082	8.65	0.9913
1.20	0.8549	3.70	0.9732	6.20	1.0123	8.70	0.9900
1.25	0.6481	3.75	0.9509	6.25	1.0161	8.75	0.9900
1.30	0.4901	3.80	0.9386	6.30	1.0206	8.80	0.9919
1.35	0.3951	3.85	0.9409	6.35	1.0249	8.85	0.9954
1.40	0.3538	3.90	0.9562	6.40	1.0277	8.90	0.9995
1.45	0.3412	3.95	0.9783	6.45	1.0274	8.95	1.0034
1.50	0.3313	4.00	0.9987	6.50	1.0233	9.00	1.0063
1.55	0.3093	4.05	1.0115	6.55	1.0164	9.05	1.0085
1.60	0.2764	4.10	1.0152	6.60	1.0091	9.10	1.0104
1.65	0.2460	4.15	1.0131	6.65	1.0042	9.15	1.0124
1.70	0.2328	4.20	1.0104	6.70	1.0035	9.20	1.0143
1.75	0.2426	4.25	1.0113	6.75	1.0073	9.25	1.0153
1.80	0.2689	4.30	1.0167	6.80	1.0141	9.30	1.0142
1.85	0.2963	4.35	1.0240	6.85	1.0211	9.35	1.0105
1.90	0.3105	4.40	1.0287	6.90	1.0262	9.40	1.0047
1.95	0.3060	4.45	1.0277	6.95	1.0282	9.45	0.9982

H_2O 100°C

R	G(R)	R	G(R)	R	G(R)	R	G(R)
2.00	0.2901	4.50	1.0205	7.00	1.0277	9.50	0.9931
2.05	0.2772	4.55	1.0099	7.05	1.0263	9.55	0.9909
2.10	0.2801	4.60	1.0003	7.10	1.0259	9.60	0.9921
2.15	0.3005	4.65	0.9953	7.15	1.0271	9.65	0.9958
2.20	0.3273	4.70	0.9959	7.20	1.0292	9.70	1.0001
2.25	0.3421	4.75	1.0003	7.25	1.0306	9.75	1.0030
2.30	0.3316	4.80	1.0050	7.30	1.0294	9.80	1.0036
2.35	0.2978	4.85	1.0065	7.35	1.0247	9.85	1.0020
2.40	0.2629	4.90	1.0036	7.40	1.0171	9.90	0.9996
2.45	0.2632	4.95	0.9974	7.45	1.0083	9.95	0.9981

INTENSITIES IN ELECTRON UNITS H_2O 150°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
0.0	0.660E 02	0.100E-01	0.111E 02	0.110E 00	-0.549E 00	0.0	0.0
0.050	0.660E 02	0.100E-01	0.111E 02	0.110E 00	-0.549E 00	-0.274E-01	0.550E-04
0.100	0.659E 02	0.100E-01	0.111E 02	0.110E 00	-0.549E 00	-0.549E-01	0.110E-03
0.150	0.657E 02	0.100E-01	0.111E 02	0.110E 00	-0.549E 00	-0.823E-01	0.166E-03
0.200	0.656E 02	0.101E-01	0.111E 02	0.110E 00	-0.548E 00	-0.110E 00	0.222E-03
0.250	0.654E 02	0.101E-01	0.111E 02	0.110E 00	-0.548E 00	-0.137E 00	0.278E-03
0.300	0.652E 02	0.101E-01	0.111E 02	0.110E 00	-0.548E 00	-0.164E 00	0.335E-03
0.350	0.649E 02	0.102E-01	0.111E 02	0.110E 00	-0.548E 00	-0.192E 00	0.392E-03
0.393	0.647E 02	0.102E-01	0.111E 02	0.110E 00	-0.547E 00	-0.210E 00	0.430E-03
0.433	0.643E 02	0.103E-01	0.112E 02	0.109E 00	-0.546E 00	-0.237E 00	0.486E-03
0.483	0.640E 02	0.103E-01	0.113E 02	0.108E 00	-0.545E 00	-0.264E 00	0.541E-03
0.533	0.636E 02	0.104E-01	0.114E 02	0.107E 00	-0.543E 00	-0.290E 00	0.593E-03
0.583	0.631E 02	0.105E-01	0.116E 02	0.105E 00	-0.541E 00	-0.316E 00	0.643E-03
0.633	0.626E 02	0.106E-01	0.118E 02	0.103E 00	-0.538E 00	-0.341E 00	0.689E-03
0.683	0.621E 02	0.107E-01	0.120E 02	0.100E 00	-0.535E 00	-0.366E 00	0.731E-03
0.733	0.616E 02	0.108E-01	0.123E 02	0.971E-01	-0.532E 00	-0.390E 00	0.769E-03
0.783	0.610E 02	0.109E-01	0.126E 02	0.937E-01	-0.528E 00	-0.413E 00	0.801E-03
0.833	0.603E 02	0.110E-01	0.129E 02	0.900E-01	-0.523E 00	-0.436E 00	0.828E-03
0.883	0.597E 02	0.112E-01	0.133E 02	0.858E-01	-0.518E 00	-0.457E 00	0.847E-03
0.933	0.590E 02	0.113E-01	0.137E 02	0.813E-01	-0.512E 00	-0.478E 00	0.859E-03
0.983	0.582E 02	0.115E-01	0.142E 02	0.764E-01	-0.505E 00	-0.497E 00	0.862E-03
1.033	0.575E 02	0.116E-01	0.147E 02	0.711E-01	-0.498E 00	-0.515E 00	0.855E-03
1.083	0.567E 02	0.118E-01	0.152E 02	0.654E-01	-0.490E 00	-0.531E 00	0.836E-03
1.133	0.560E 02	0.120E-01	0.157E 02	0.593E-01	-0.482E 00	-0.546E 00	0.805E-03
1.183	0.552E 02	0.122E-01	0.163E 02	0.528E-01	-0.473E 00	-0.560E 00	0.760E-03
1.233	0.544E 02	0.124E-01	0.169E 02	0.460E-01	-0.463E 00	-0.571E 00	0.701E-03
1.310	0.531E 02	0.127E-01	0.185E 02	0.503E-01	-0.439E 00	-0.575E 00	0.835E-03
1.387	0.518E 02	0.130E-01	0.209E 02	0.564E-01	-0.404E 00	-0.560E 00	0.102E-02
1.464	0.504E 02	0.134E-01	0.235E 02	0.636E-01	-0.361E 00	-0.528E 00	0.125E-02
1.541	0.491E 02	0.138E-01	0.267E 02	0.720E-01	-0.309E 00	-0.477E 00	0.154E-02
1.618	0.477E 02	0.143E-01	0.308E 02	0.828E-01	-0.241E 00	-0.390E 00	0.191E-02
1.695	0.464E 02	0.147E-01	0.356E 02	0.953E-01	-0.159E 00	-0.269E 00	0.238E-02
1.771	0.450E 02	0.152E-01	0.389E 02	0.104E 00	-0.935E-01	-0.166E 00	0.280E-02
1.848	0.436E 02	0.157E-01	0.440E 02	0.118E 00	0.607E-02	0.112E-01	0.342E-02
1.925	0.422E 02	0.163E-01	0.470E 02	0.125E 00	0.773E-01	0.149E 00	0.393E-02
2.002	0.408E 02	0.169E-01	0.514E 02	0.137E 00	0.179E 00	0.358E 00	0.464E-02
2.078	0.395E 02	0.175E-01	0.554E 02	0.148E 00	0.279E 00	0.581E 00	0.538E-02
2.155	0.382E 02	0.182E-01	0.597E 02	0.144E 00	0.283E 00	0.609E 00	0.563E-02
2.231	0.369E 02	0.189E-01	0.530E 02	0.142E 00	0.305E 00	0.680E 00	0.599E-02
2.308	0.356E 02	0.196E-01	0.509E 02	0.137E 00	0.299E 00	0.691E 00	0.619E-02
2.384	0.343E 02	0.204E-01	0.484E 02	0.131E 00	0.288E 00	0.687E 00	0.637E-02
2.461	0.331E 02	0.213E-01	0.455E 02	0.123E 00	0.265E 00	0.652E 00	0.646E-02
2.537	0.319E 02	0.222E-01	0.429E 02	0.117E 00	0.246E 00	0.624E 00	0.659E-02
2.614	0.307E 02	0.231E-01	0.407E 02	0.111E 00	0.230E 00	0.600E 00	0.673E-02
2.690	0.296E 02	0.241E-01	0.368E 02	0.102E 00	0.174E 00	0.467E 00	0.660E-02
2.766	0.285E 02	0.251E-01	0.336E 02	0.940E-01	0.129E 00	0.354E 00	0.652E-02
2.842	0.274E 02	0.261E-01	0.318E 02	0.898E-01	0.115E 00	0.326E 00	0.667E-02
2.918	0.264E 02	0.273E-01	0.292E 02	0.834E-01	0.760E-01	0.222E 00	0.663E-02
2.994	0.254E 02	0.284E-01	0.261E 02	0.757E-01	0.192E-01	0.575E-01	0.645E-02
3.070	0.244E 02	0.297E-01	0.249E 02	0.738E-01	0.144E-01	0.442E-01	0.673E-02
3.146	0.235E 02	0.310E-01	0.227E 02	0.681E-01	-0.240E-01	-0.756E-01	0.664E-02
3.222	0.226E 02	0.323E-01	0.204E 02	0.626E-01	-0.724E-01	-0.233E 00	0.653E-02
3.298	0.217E 02	0.338E-01	0.176E 02	0.560E-01	-0.138E 00	-0.456E 00	0.624E-02
3.374	0.209E 02	0.353E-01	0.167E 02	0.536E-01	-0.146E 00	-0.493E 00	0.638E-02
3.525	0.193E 02	0.385E-01	0.152E 02	0.443E-01	-0.157E 00	-0.553E 00	0.601E-02
3.676	0.178E 02	0.420E-01	0.141E 02	0.422E-01	-0.155E 00	-0.571E 00	0.652E-02
3.827	0.164E 02	0.458E-01	0.133E 02	0.409E-01	-0.142E 00	-0.545E 00	0.717E-02

H_2O 150°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
3.978	0.152E 02	0.499E-01	0.132E 02	0.410E-01	-0.995E-01	-0.396E 00	0.814E-02
4.128	0.141E 02	0.543E-01	0.132E 02	0.412E-01	-0.456E-01	-0.188E 00	0.924E-02
4.278	0.130E 02	0.591E-01	0.124E 02	0.395E-01	-0.365E-01	-0.156E 00	0.993E-02
4.427	0.121E 02	0.641E-01	0.121E 02	0.389E-01	0.861E-03	0.381E-02	0.110E-01
4.576	0.113E 02	0.694E-01	0.112E 02	0.368E-01	-0.778E-02	-0.356E-01	0.117E-01
4.725	0.105E 02	0.753E-01	0.107E 02	0.357E-01	0.152E-01	0.720E-01	0.127E-01
4.874	0.976E 01	0.814E-01	0.989E 01	0.340E-01	0.113E-01	0.549E-01	0.135E-01
5.022	0.911E 01	0.877E-01	0.919E 01	0.324E-01	0.729E-02	0.366E-01	0.143E-01
5.170	0.851E 01	0.946E-01	0.849E 01	0.309E-01	-0.223E-02	-0.115E-01	0.151E-01
5.317	0.797E 01	0.102E 00	0.767E 01	0.289E-01	-0.312E-01	-0.166E 00	0.156E-01
5.464	0.750E 01	0.109E 00	0.719E 01	0.278E-01	-0.337E-01	-0.184E 00	0.166E-01
5.610	0.705E 01	0.117E 00	0.656E 01	0.263E-01	-0.575E-01	-0.322E 00	0.172E-01
5.757	0.665E 01	0.125E 00	0.592E 01	0.248E-01	-0.908E-01	-0.523E 00	0.178E-01
5.902	0.628E 01	0.133E 00	0.570E 01	0.241E-01	-0.767E-01	-0.452E 00	0.189E-01
6.047	0.595E 01	0.141E 00	0.548E 01	0.235E-01	-0.665E-01	-0.402E 00	0.201E-01
6.192	0.564E 01	0.150E 00	0.530E 01	0.230E-01	-0.613E-01	-0.378E 00	0.213E-01
6.337	0.536E 01	0.158E 00	0.526E 01	0.228E-01	-0.165E-01	-0.104E 00	0.229E-01
6.480	0.511E 01	0.167E 00	0.512E 01	0.224E-01	0.147E-02	0.955E-02	0.243E-01
6.624	0.488E 01	0.176E 00	0.490E 01	0.215E-01	-0.131E-01	-0.870E-01	0.251E-01
6.766	0.466E 01	0.185E 00	0.490E 01	0.214E-01	0.435E-01	0.294E 00	0.268E-01
6.909	0.447E 01	0.194E 00	0.467E 01	0.203E-01	0.376E-01	0.259E 00	0.273E-01
7.051	0.430E 01	0.203E 00	0.458E 01	0.201E-01	0.568E-01	0.400E 00	0.289E-01
7.192	0.413E 01	0.213E 00	0.428E 01	0.192E-01	0.309E-01	0.222E 00	0.294E-01
7.332	0.398E 01	0.222E 00	0.407E 01	0.115E-01	0.187E-01	0.137E 00	0.188E-01
7.473	0.384E 01	0.231E 00	0.395E 01	0.112E-01	0.240E-01	0.179E 00	0.193E-01
7.612	0.372E 01	0.240E 00	0.368E 01	0.105E-01	-0.900E-02	-0.685E-01	0.193E-01
7.751	0.360E 01	0.249E 00	0.363E 01	0.102E-01	0.882E-02	0.684E-01	0.197E-01
7.890	0.349E 01	0.258E 00	0.346E 01	0.971E-02	-0.741E-02	-0.585E-01	0.197E-01
8.027	0.339E 01	0.266E 00	0.336E 01	0.932E-02	-0.849E-02	-0.681E-01	0.199E-01
8.164	0.329E 01	0.275E 00	0.324E 01	0.894E-02	-0.139E-01	-0.113E 00	0.201E-01
8.301	0.321E 01	0.284E 00	0.323E 01	0.870E-02	0.652E-02	0.542E-01	0.205E-01
8.437	0.313E 01	0.292E 00	0.310E 01	0.830E-02	-0.746E-02	-0.629E-01	0.205E-01
8.572	0.305E 01	0.300E 00	0.307E 01	0.806E-02	0.535E-02	0.459E-01	0.207E-01
8.707	0.298E 01	0.309E 00	0.300E 01	0.778E-02	0.583E-02	0.508E-01	0.209E-01
8.841	0.291E 01	0.317E 00	0.293E 01	0.750E-02	0.480E-02	0.424E-01	0.210E-01
8.974	0.285E 01	0.324E 00	0.289E 01	0.727E-02	0.119E-01	0.107E 00	0.211E-01
9.107	0.279E 01	0.332E 00	0.291E 01	0.699E-02	0.410E-02	0.373E-01	0.211E-01
9.239	0.274E 01	0.340E 00	0.277E 01	0.678E-02	0.104E-01	0.962E-01	0.213E-01
9.370	0.269E 01	0.347E 00	0.271E 01	0.655E-02	0.855E-02	0.801E-01	0.213E-01
9.500	0.264E 01	0.355E 00	0.267E 01	0.634E-02	0.110E-01	0.105E 00	0.214E-01
9.630	0.259E 01	0.362E 00	0.269E 01	0.609E-02	-0.280E-02	-0.270E-01	0.212E-01
9.759	0.255E 01	0.369E 00	0.253E 01	0.589E-02	-0.803E-02	-0.784E-01	0.212E-01
9.887	0.251E 01	0.376E 00	0.249E 01	0.572E-02	-0.446E-02	-0.441E-01	0.212E-01
10.015	0.247E 01	0.382E 00	0.246E 01	0.555E-02	-0.210E-02	-0.210E-01	0.213E-01
10.142	0.243E 01	0.389E 00	0.240E 01	0.537E-02	-0.103E-01	-0.105E 00	0.212E-01
10.268	0.239E 01	0.396E 00	0.238E 01	0.523E-02	-0.613E-02	-0.630E-01	0.213E-01
10.393	0.236E 01	0.403E 00	0.235E 01	0.510E-02	-0.222E-02	-0.231E-01	0.213E-01
10.517	0.233E 01	0.409E 00	0.229E 01	0.493E-02	-0.125E-01	-0.131E 00	0.212E-01
10.641	0.229E 01	0.416E 00	0.228E 01	0.484E-02	-0.765E-02	-0.814E-01	0.214E-01
10.764	0.226E 01	0.422E 00	0.224E 01	0.472E-02	-0.920E-02	-0.990E-01	0.215E-01
10.886	0.224E 01	0.429E 00	0.221E 01	0.464E-02	-0.933E-02	-0.102E 00	0.216E-01
11.007	0.221E 01	0.435E 00	0.220E 01	0.455E-02	-0.564E-02	-0.621E-01	0.218E-01
11.127	0.218E 01	0.442E 00	0.216E 01	0.445E-02	-0.760E-02	-0.845E-01	0.219E-01
11.247	0.215E 01	0.448E 00	0.215E 01	0.439E-02	-0.327E-02	-0.367E-01	0.221E-01
11.366	0.213E 01	0.454E 00	0.212E 01	0.429E-02	-0.579E-02	-0.657E-01	0.221E-01
11.483	0.210E 01	0.460E 00	0.210E 01	0.423E-02	-0.680E-03	-0.781E-02	0.223E-01
11.600	0.208E 01	0.466E 00	0.208E 01	0.416E-02	0.132E-02	0.153E-01	0.225E-01
11.716	0.206E 01	0.472E 00	0.205E 01	0.408E-02	-0.222E-02	-0.260E-01	0.225E-01
11.831	0.203E 01	0.477E 00	0.204E 01	0.403E-02	0.455E-02	0.539E-01	0.228E-01
11.946	0.201E 01	0.483E 00	0.202E 01	0.396E-02	0.417E-02	0.498E-01	0.229E-01
12.059	0.199E 01	0.488E 00	0.199E 01	0.389E-02	-0.132E-03	-0.159E-02	0.229E-01
12.171	0.197E 01	0.494E 00	0.196E 01	0.382E-02	-0.344E-02	-0.418E-01	0.230E-01
12.283	0.195E 01	0.499E 00	0.194E 01	0.377E-02	-0.265E-02	-0.326E-01	0.231E-01
12.393	0.193E 01	0.505E 00	0.192E 01	0.372E-02	-0.274E-02	-0.340E-01	0.233E-01
12.503	0.191E 01	0.510E 00	0.191E 01	0.367E-02	0.984E-04	0.120E-02	0.234E-01
12.611	0.189E 01	0.516E 00	0.188E 01	0.361E-02	-0.640E-02	-0.807E-01	0.235E-01
12.719	0.187E 01	0.522E 00	0.186E 01	0.358E-02	-0.498E-02	-0.633E-01	0.237E-01
12.826	0.185E 01	0.528E 00	0.184E 01	0.353E-02	-0.641E-02	-0.822E-01	0.239E-01
12.932	0.183E 01	0.534E 00	0.183E 01	0.350E-02	-0.315E-02	-0.407E-01	0.241E-01
13.036	0.181E 01	0.540E 00	0.181E 01	0.346E-02	-0.317E-02	-0.413E-01	0.244E-01
13.140	0.179E 01	0.546E 00	0.179E 01	0.343E-02	-0.319E-02	-0.418E-01	0.246E-01
13.243	0.178E 01	0.552E 00	0.177E 01	0.340E-02	-0.154E-02	-0.204E-01	0.249E-01
13.345	0.176E 01	0.558E 00	0.175E 01	0.337E-02	-0.278E-02	-0.371E-01	0.251E-01
13.445	0.174E 01	0.565E 00	0.173E 01	0.334E-02	-0.343E-02	-0.461E-01	0.253E-01
13.545	0.172E 01	0.571E 00	0.172E 01	0.332E-02	-0.616E-03	-0.835E-02	0.257E-01
13.644	0.170E 01	0.577E 00	0.170E 01	0.329E-02	-0.322E-03	-0.439E-02	0.259E-01

H_2O 150°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
13.741	0.169E 01	0.583E 00	0.169E 01	0.327E-02	0.723E-03	0.994E-02	0.262E-01
13.838	0.167E 01	0.589E 00	0.167E 01	0.324E-02	0.249E-02	0.344E-01	0.264E-01
13.933	0.165E 01	0.595E 00	0.165E 01	0.321E-02	-0.666E-03	-0.929E-02	0.266E-01
14.028	0.164E 01	0.600E 00	0.164E 01	0.320E-02	0.514E-02	0.721E-01	0.269E-01
14.214	0.160E 01	0.612E 00	0.161E 01	0.315E-02	0.357E-02	0.507E-01	0.274E-01
14.395	0.158E 01	0.623E 00	0.159E 01	0.311E-02	0.583E-02	0.840E-01	0.278E-01
14.572	0.155E 01	0.634E 00	0.155E 01	0.305E-02	0.120E-02	0.175E-01	0.282E-01
14.744	0.152E 01	0.645E 00	0.152E 01	0.300E-02	-0.349E-02	-0.514E-01	0.285E-01
14.913	0.150E 01	0.656E 00	0.150E 01	0.297E-02	0.380E-03	0.566E-02	0.291E-01
15.076	0.148E 01	0.668E 00	0.148E 01	0.293E-02	-0.506E-03	-0.763E-02	0.295E-01
15.235	0.145E 01	0.679E 00	0.145E 01	0.290E-02	-0.199E-02	-0.303E-01	0.300E-01
15.389	0.143E 01	0.691E 00	0.143E 01	0.287E-02	-0.182E-02	-0.279E-01	0.305E-01
15.539	0.140E 01	0.702E 00	0.140E 01	0.284E-02	-0.354E-02	-0.550E-01	0.309E-01
15.684	0.138E 01	0.713E 00	0.138E 01	0.281E-02	-0.142E-02	-0.222E-01	0.314E-01
15.824	0.136E 01	0.723E 00	0.136E 01	0.278E-02	-0.192E-02	-0.304E-01	0.318E-01
15.959	0.135E 01	0.732E 00	0.134E 01	0.275E-02	-0.110E-02	-0.175E-01	0.322E-01

RADIAL DISTRIBUTION FUNCTIONS TO 10 A

H_2O 150°C

R	G(R)	R	G(R)	R	G(R)	R	G(R)
0.0	0.0	2.50	0.3649	5.00	1.0005	7.50	1.0093
0.05	-4.1931	2.55	0.5075	5.05	0.9905	7.55	1.0079
0.10	-3.7417	2.60	0.7115	5.10	0.9780	7.60	1.0026
0.15	-3.0951	2.65	0.9518	5.15	0.9666	7.65	0.9941
0.20	-2.3773	2.70	1.1917	5.20	0.9595	7.70	0.9844
0.25	-1.7059	2.75	1.3954	5.25	0.9585	7.75	0.9764
0.30	-1.1618	2.80	1.5388	5.30	0.9633	7.80	0.9722
0.35	-0.7746	2.85	1.6154	5.35	0.9714	7.85	0.9728
0.40	-0.5254	2.90	1.6343	5.40	0.9792	7.90	0.9777
0.45	-0.3634	2.95	1.6135	5.45	0.9835	7.95	0.9851
0.50	-0.2292	3.00	1.5713	5.50	0.9829	8.00	0.9929
0.55	-0.0741	3.05	1.5194	5.55	0.9782	8.05	0.9994
0.60	0.1298	3.10	1.4621	5.60	0.9721	8.10	1.0038
0.65	0.3873	3.15	1.3980	5.65	0.9677	8.15	1.0063
0.70	0.6857	3.20	1.3256	5.70	0.9672	8.20	1.0074
0.75	1.0003	3.25	1.2470	5.75	0.9709	8.25	1.0076
0.80	1.3001	3.30	1.1691	5.80	0.9773	8.30	1.0071
0.85	1.5515	3.35	1.1018	5.85	0.9839	8.35	1.0056
0.90	1.7221	3.40	1.0540	5.90	0.9889	8.40	1.0031
0.95	1.7862	3.45	1.0302	5.95	0.9918	8.45	0.9995
1.00	1.7317	3.50	1.0284	6.00	0.9940	8.50	0.9954
1.05	1.5661	3.55	1.0418	6.05	0.9977	8.55	0.9918
1.10	1.3178	3.60	1.0613	6.10	1.0044	8.60	0.9895
1.15	1.0309	3.65	1.0787	6.15	1.0142	8.65	0.9891
1.20	0.7543	3.70	1.0890	6.20	1.0254	8.70	0.9902
1.25	0.5277	3.75	1.0907	6.25	1.0348	8.75	0.9923
1.30	0.3712	3.80	1.0847	6.30	1.0397	8.80	0.9943
1.35	0.2924	3.85	1.0729	6.35	1.0389	8.85	0.9958
1.40	0.2420	3.90	1.0570	6.40	1.0333	8.90	0.9968
1.45	0.2250	3.95	1.0378	6.45	1.0255	8.95	0.9978
1.50	0.2127	4.00	1.0162	6.50	1.0188	9.00	0.9997
1.55	0.1993	4.05	0.9935	6.55	1.0151	9.05	1.0030
1.60	0.1907	4.10	0.9716	6.60	1.0149	9.10	1.0074
1.65	0.1973	4.15	0.9530	6.65	1.0165	9.15	1.0120
1.70	0.2244	4.20	0.9400	6.70	1.0177	9.20	1.0155
1.75	0.2670	4.25	0.9335	6.75	1.0165	9.25	1.0168
1.80	0.3102	4.30	0.9330	6.80	1.0126	9.30	1.0155
1.85	0.3367	4.35	0.9368	6.85	1.0071	9.35	1.0118
1.90	0.3354	4.40	0.9424	6.90	1.0021	9.40	1.0071
1.95	0.3075	4.45	0.9477	6.95	0.9995	9.45	1.0027
2.00	0.2667	4.50	0.9518	7.00	0.9998	9.50	0.9997
2.05	0.2320	4.55	0.9547	7.05	1.0023	9.55	0.9984
2.10	0.2180	4.60	0.9576	7.10	1.0053	9.60	0.9982
2.15	0.2278	4.65	0.9619	7.15	1.0070	9.65	0.9981
2.20	0.2519	4.70	0.9685	7.20	1.0067	9.70	0.9972
2.25	0.2740	4.75	0.9776	7.25	1.0051	9.75	0.9951
2.30	0.2815	4.80	0.9880	7.30	1.0036	9.80	0.9924
2.35	0.2744	4.85	0.9977	7.35	1.0035	9.85	0.9903
2.40	0.2684	4.90	1.0042	7.40	1.0052	9.90	0.9900
2.45	0.2899	4.95	1.0054	7.45	1.0078	9.95	0.9922

INTENSITIES IN ELECTRON UNITS H_2O 200°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
0.0	0.660E 02	0.100E-01	0.153E 02	0.150E 00	-0.507E 00	0.0	0.0
0.050	0.660E 02	0.100E-01	0.153E 02	0.150E 00	-0.507E 00	-0.254E-01	0.751E-04
0.100	0.659E 02	0.100E-01	0.153E 02	0.150E 00	-0.507E 00	-0.507E-01	0.150E-03
0.150	0.657E 02	0.100E-01	0.153E 02	0.150E 00	-0.507E 00	-0.760E-01	0.226E-03
0.200	0.656E 02	0.101E-01	0.153E 02	0.150E 00	-0.507E 00	-0.101E 00	0.302E-03
0.250	0.654E 02	0.101E-01	0.153E 02	0.150E 00	-0.506E 00	-0.127E 00	0.379E-03
0.300	0.652E 02	0.101E-01	0.153E 02	0.150E 00	-0.506E 00	-0.152E 00	0.456E-03
0.350	0.649E 02	0.102E-01	0.153E 02	0.150E 00	-0.506E 00	-0.177E 00	0.535E-03
0.383	0.647E 02	0.102E-01	0.153E 02	0.150E 00	-0.505E 00	-0.194E 00	0.587E-03
0.433	0.643E 02	0.103E-01	0.154E 02	0.149E 00	-0.504E 00	-0.218E 00	0.663E-03
0.483	0.640E 02	0.103E-01	0.155E 02	0.147E 00	-0.502E 00	-0.242E 00	0.737E-03
0.533	0.636E 02	0.104E-01	0.157E 02	0.145E 00	-0.499E 00	-0.266E 00	0.807E-03
0.583	0.631E 02	0.105E-01	0.159E 02	0.143E 00	-0.496E 00	-0.289E 00	0.874E-03
0.633	0.626E 02	0.106E-01	0.162E 02	0.139E 00	-0.492E 00	-0.312E 00	0.936E-03
0.683	0.621E 02	0.107E-01	0.165E 02	0.136E 00	-0.488E 00	-0.333E 00	0.992E-03
0.733	0.616E 02	0.108E-01	0.168E 02	0.132E 00	-0.483E 00	-0.354E 00	0.104E-02
0.783	0.610E 02	0.109E-01	0.173E 02	0.127E 00	-0.477E 00	-0.374E 00	0.108E-02
0.833	0.603E 02	0.110E-01	0.177E 02	0.121E 00	-0.470E 00	-0.392E 00	0.112E-02
0.883	0.597E 02	0.112E-01	0.182E 02	0.115E 00	-0.463E 00	-0.409E 00	0.114E-02
0.933	0.589E 02	0.113E-01	0.188E 02	0.109E 00	-0.455E 00	-0.424E 00	0.115E-02
0.983	0.582E 02	0.115E-01	0.194E 02	0.102E 00	-0.446E 00	-0.438E 00	0.115E-02
1.033	0.575E 02	0.116E-01	0.200E 02	0.942E-01	-0.436E 00	-0.450E 00	0.113E-02
1.083	0.567E 02	0.118E-01	0.207E 02	0.860E-01	-0.425E 00	-0.461E 00	0.110E-02
1.133	0.560E 02	0.120E-01	0.214E 02	0.773E-01	-0.414E 00	-0.469E 00	0.105E-02
1.183	0.552E 02	0.122E-01	0.222E 02	0.680E-01	-0.401E 00	-0.474E 00	0.979E-03
1.233	0.544E 02	0.124E-01	0.231E 02	0.582E-01	-0.387E 00	-0.478E 00	0.887E-03
1.310	0.531E 02	0.127E-01	0.248E 02	0.626E-01	-0.360E 00	-0.471E 00	0.104E-02
1.387	0.518E 02	0.130E-01	0.268E 02	0.679E-01	-0.325E 00	-0.451E 00	0.123E-02
1.464	0.504E 02	0.134E-01	0.292E 02	0.739E-01	-0.285E 00	-0.417E 00	0.145E-02
1.541	0.491E 02	0.138E-01	0.321E 02	0.810E-01	-0.235E 00	-0.362E 00	0.173E-02
1.618	0.477E 02	0.143E-01	0.354E 02	0.892E-01	-0.176E 00	-0.285E 00	0.206E-02
1.695	0.464E 02	0.147E-01	0.399E 02	0.100E 00	-0.951E-01	-0.161E 00	0.250E-02
1.771	0.450E 02	0.152E-01	0.444E 02	0.111E 00	-0.925E-02	-0.164E-01	0.300E-02
1.848	0.436E 02	0.157E-01	0.480E 02	0.120E 00	0.688E-01	0.127E 00	0.349E-02
1.926	0.422E 02	0.163E-01	0.514E 02	0.129E 00	0.149E 00	0.287E 00	0.403E-02
2.002	0.408E 02	0.169E-01	0.555E 02	0.139E 00	0.248E 00	0.497E 00	0.469E-02
2.078	0.395E 02	0.175E-01	0.555E 02	0.139E 00	0.280E 00	0.583E 00	0.506E-02
2.155	0.382E 02	0.182E-01	0.573E 02	0.143E 00	0.349E 00	0.751E 00	0.562E-02
2.231	0.369E 02	0.189E-01	0.560E 02	0.140E 00	0.361E 00	0.805E 00	0.592E-02
2.308	0.356E 02	0.196E-01	0.553E 02	0.139E 00	0.388E 00	0.895E 00	0.630E-02
2.384	0.343E 02	0.204E-01	0.532E 02	0.134E 00	0.385E 00	0.917E 00	0.653E-02
2.461	0.331E 02	0.213E-01	0.492E 02	0.125E 00	0.343E 00	0.845E 00	0.654E-02
2.537	0.319E 02	0.222E-01	0.461E 02	0.118E 00	0.315E 00	0.799E 00	0.662E-02
2.614	0.307E 02	0.231E-01	0.440E 02	0.113E 00	0.308E 00	0.804E 00	0.681E-02
2.690	0.296E 02	0.241E-01	0.398E 02	0.103E 00	0.245E 00	0.659E 00	0.665E-02
2.766	0.285E 02	0.251E-01	0.364E 02	0.949E-01	0.198E 00	0.549E 00	0.658E-02
2.843	0.274E 02	0.261E-01	0.322E 02	0.849E-01	0.124E 00	0.352E 00	0.631E-02
2.919	0.264E 02	0.273E-01	0.298E 02	0.793E-01	0.925E-01	0.270E 00	0.631E-02
2.994	0.254E 02	0.284E-01	0.271E 02	0.729E-01	0.473E-01	0.142E 00	0.621E-02
3.070	0.244E 02	0.297E-01	0.242E 02	0.661E-01	-0.773E-02	-0.237E-01	0.602E-02
3.146	0.235E 02	0.310E-01	0.221E 02	0.611E-01	-0.435E-01	-0.137E 00	0.596E-02
3.222	0.226E 02	0.323E-01	0.204E 02	0.571E-01	-0.704E-01	-0.227E 00	0.595E-02
3.298	0.217E 02	0.338E-01	0.187E 02	0.530E-01	-0.101E 00	-0.334E 00	0.591E-02
3.374	0.209E 02	0.353E-01	0.173E 02	0.496E-01	-0.127E 00	-0.429E 00	0.590E-02
3.450	0.200E 02	0.369E-01	0.162E 02	0.470E-01	-0.141E 00	-0.487E 00	0.598E-02
3.525	0.193E 02	0.385E-01	0.155E 02	0.454E-01	-0.144E 00	-0.507E 00	0.615E-02
3.601	0.185E 02	0.402E-01	0.147E 02	0.433E-01	-0.154E 00	-0.555E 00	0.627E-02
3.676	0.178E 02	0.420E-01	0.144E 02	0.427E-01	-0.141E 00	-0.517E 00	0.659E-02
3.752	0.171E 02	0.439E-01	0.137E 02	0.409E-01	-0.148E 00	-0.556E 00	0.673E-02
3.827	0.164E 02	0.458E-01	0.135E 02	0.403E-01	-0.135E 00	-0.518E 00	0.706E-02
3.902	0.158E 02	0.478E-01	0.132E 02	0.396E-01	-0.125E 00	-0.486E 00	0.732E-02
3.978	0.152E 02	0.499E-01	0.130E 02	0.389E-01	-0.109E 00	-0.429E 00	0.771E-02
4.053	0.146E 02	0.520E-01	0.130E 02	0.389E-01	-0.883E-01	-0.350E 00	0.820E-02
4.128	0.141E 02	0.543E-01	0.129E 02	0.387E-01	-0.635E-01	-0.262E 00	0.868E-02
4.203	0.135E 02	0.566E-01	0.129E 02	0.386E-01	-0.346E-01	-0.145E 00	0.918E-02
4.278	0.130E 02	0.591E-01	0.127E 02	0.382E-01	-0.172E-01	-0.735E-01	0.965E-02
4.427	0.121E 02	0.641E-01	0.123E 02	0.369E-01	0.101E-01	0.447E-01	0.964E-02
4.576	0.113E 02	0.694E-01	0.117E 02	0.327E-01	0.336E-01	0.154E 00	0.104E-01
4.725	0.105E 02	0.753E-01	0.109E 02	0.307E-01	0.313E-01	0.148E 00	0.109E-01
4.874	0.975E 01	0.814E-01	0.101E 02	0.288E-01	0.252E-01	0.123E 00	0.114E-01
5.022	0.911E 01	0.877E-01	0.934E 01	0.272E-01	0.207E-01	0.104E 00	0.120E-01
5.170	0.851E 01	0.946E-01	0.850E 01	0.253E-01	-0.121E-02	-0.625E-02	0.124E-01

H_2O 200°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
5.317	0.797E 01	0.102E 00	0.768E 01	0.236E-01	-0.295E-01	-0.157E 00	0.128E-01
5.464	0.750E 01	0.109E 00	0.700E 01	0.221E-01	-0.537E-01	-0.293E 00	0.132E-01
5.610	0.705E 01	0.117E 00	0.646E 01	0.208E-01	-0.690E-01	-0.387E 00	0.136E-01
5.757	0.665E 01	0.125E 00	0.611E 01	0.198E-01	-0.665E-01	-0.383E 00	0.142E-01
5.902	0.628E 01	0.133E 00	0.583E 01	0.190E-01	-0.605E-01	-0.357E 00	0.149E-01
6.047	0.595E 01	0.141E 00	0.559E 01	0.182E-01	-0.512E-01	-0.310E 00	0.155E-01
6.192	0.564E 01	0.150E 00	0.547E 01	0.176E-01	-0.259E-01	-0.160E 00	0.163E-01
6.337	0.536E 01	0.158E 00	0.534E 01	0.170E-01	-0.380E-02	-0.241E-01	0.170E-01
6.480	0.511E 01	0.167E 00	0.520E 01	0.163E-01	0.142E-01	0.918E-01	0.177E-01
6.624	0.488E 01	0.176E 00	0.502E 01	0.157E-01	0.243E-01	0.161E 00	0.183E-01
6.766	0.466E 01	0.185E 00	0.490E 01	0.152E-01	0.440E-01	0.298E 00	0.190E-01
6.909	0.447E 01	0.194E 00	0.470E 01	0.145E-01	0.437E-01	0.302E 00	0.195E-01
7.051	0.430E 01	0.203E 00	0.446E 01	0.137E-01	0.322E-01	0.227E 00	0.196E-01
7.192	0.413E 01	0.213E 00	0.421E 01	0.130E-01	0.173E-01	0.124E 00	0.198E-01
7.332	0.398E 01	0.222E 00	0.402E 01	0.121E-01	0.774E-02	0.568E-01	0.198E-01
7.473	0.384E 01	0.231E 00	0.388E 01	0.115E-01	0.711E-02	0.531E-01	0.199E-01
7.612	0.372E 01	0.240E 00	0.373E 01	0.925E-02	0.333E-02	0.253E-01	0.169E-01
7.751	0.360E 01	0.249E 00	0.360E 01	0.885E-02	0.920E-03	0.713E-02	0.171E-01
7.890	0.349E 01	0.258E 00	0.348E 01	0.847E-02	-0.178E-02	-0.141E-01	0.172E-01
8.027	0.339E 01	0.266E 00	0.338E 01	0.813E-02	-0.154E-02	-0.124E-01	0.174E-01
8.164	0.329E 01	0.275E 00	0.328E 01	0.782E-02	-0.325E-02	-0.265E-01	0.176E-01
8.301	0.321E 01	0.284E 00	0.321E 01	0.756E-02	0.172E-02	0.142E-01	0.178E-01
8.437	0.313E 01	0.292E 00	0.312E 01	0.727E-02	-0.582E-03	-0.491E-02	0.179E-01
8.572	0.305E 01	0.300E 00	0.309E 01	0.711E-02	0.111E-01	0.954E-01	0.183E-01
8.707	0.298E 01	0.309E 00	0.300E 01	0.687E-02	0.531E-02	0.462E-01	0.185E-01
8.841	0.291E 01	0.317E 00	0.293E 01	0.668E-02	0.434E-02	0.384E-01	0.187E-01
8.974	0.285E 01	0.324E 00	0.288E 01	0.652E-02	0.840E-02	0.754E-01	0.190E-01
9.107	0.279E 01	0.332E 00	0.281E 01	0.633E-02	0.671E-02	0.611E-01	0.191E-01
9.239	0.274E 01	0.340E 00	0.276E 01	0.615E-02	0.793E-02	0.733E-01	0.193E-01
9.370	0.269E 01	0.347E 00	0.271E 01	0.597E-02	0.671E-02	0.629E-01	0.194E-01
9.500	0.264E 01	0.355E 00	0.266E 01	0.581E-02	0.856E-02	0.813E-01	0.196E-01
9.630	0.259E 01	0.362E 00	0.260E 01	0.565E-02	0.407E-02	0.392E-01	0.197E-01
9.759	0.255E 01	0.369E 00	0.256E 01	0.550E-02	0.364E-02	0.355E-01	0.198E-01
9.887	0.251E 01	0.376E 00	0.251E 01	0.537E-02	0.119E-02	0.117E-01	0.200E-01
10.015	0.247E 01	0.382E 00	0.246E 01	0.524E-02	-0.189E-02	-0.189E-01	0.201E-01
10.142	0.243E 01	0.389E 00	0.240E 01	0.394E-02	-0.101E-01	-0.102E 00	0.156E-01
10.268	0.239E 01	0.396E 00	0.236E 01	0.384E-02	-0.141E-01	-0.145E 00	0.156E-01
10.393	0.236E 01	0.403E 00	0.232E 01	0.377E-02	-0.136E-01	-0.142E 00	0.158E-01
10.517	0.233E 01	0.409E 00	0.230E 01	0.371E-02	-0.962E-02	-0.101E 00	0.159E-01
10.641	0.229E 01	0.416E 00	0.227E 01	0.363E-02	-0.116E-01	-0.123E 00	0.161E-01
10.764	0.226E 01	0.422E 00	0.225E 01	0.358E-02	-0.741E-02	-0.798E-01	0.163E-01
10.886	0.224E 01	0.429E 00	0.221E 01	0.350E-02	-0.100E-01	-0.109E 00	0.163E-01
11.007	0.221E 01	0.435E 00	0.220E 01	0.346E-02	-0.271E-02	-0.298E-01	0.166E-01
11.127	0.219E 01	0.442E 00	0.218E 01	0.343E-02	0.787E-04	0.876E-03	0.168E-01
11.247	0.215E 01	0.448E 00	0.215E 01	0.338E-02	-0.739E-03	-0.831E-02	0.170E-01
11.366	0.213E 01	0.454E 00	0.213E 01	0.334E-02	0.199E-02	0.226E-01	0.172E-01
11.483	0.210E 01	0.460E 00	0.211E 01	0.331E-02	0.490E-02	0.563E-01	0.175E-01
11.600	0.208E 01	0.466E 00	0.209E 01	0.326E-02	0.377E-02	0.437E-01	0.176E-01
11.716	0.206E 01	0.472E 00	0.206E 01	0.322E-02	0.226E-02	0.265E-01	0.178E-01
11.831	0.203E 01	0.477E 00	0.203E 01	0.318E-02	0.934E-03	0.110E-01	0.180E-01
11.946	0.201E 01	0.483E 00	0.201E 01	0.314E-02	-0.207E-04	-0.248E-03	0.181E-01
12.059	0.199E 01	0.488E 00	0.199E 01	0.310E-02	-0.522E-04	-0.629E-03	0.183E-01
12.171	0.197E 01	0.494E 00	0.197E 01	0.306E-02	-0.120E-02	-0.146E-01	0.184E-01
12.283	0.195E 01	0.499E 00	0.194E 01	0.301E-02	-0.539E-02	-0.662E-01	0.185E-01
12.393	0.193E 01	0.505E 00	0.192E 01	0.298E-02	-0.416E-02	-0.516E-01	0.187E-01
12.503	0.191E 01	0.510E 00	0.190E 01	0.295E-02	-0.559E-02	-0.699E-01	0.188E-01
12.611	0.189E 01	0.516E 00	0.189E 01	0.294E-02	0.823E-03	0.104E-01	0.191E-01
12.719	0.187E 01	0.522E 00	0.186E 01	0.289E-02	-0.558E-02	-0.709E-01	0.192E-01
12.826	0.185E 01	0.528E 00	0.185E 01	0.288E-02	-0.252E-02	-0.323E-01	0.195E-01
12.932	0.183E 01	0.534E 00	0.183E 01	0.285E-02	-0.215E-02	-0.277E-01	0.197E-01
13.036	0.181E 01	0.540E 00	0.182E 01	0.284E-02	0.312E-02	0.407E-01	0.200E-01
13.140	0.179E 01	0.546E 00	0.181E 01	0.284E-02	0.775E-02	0.102E 00	0.203E-01
13.243	0.178E 01	0.552E 00	0.178E 01	0.280E-02	0.610E-03	0.807E-02	0.204E-01
13.345	0.176E 01	0.558E 00	0.176E 01	0.278E-02	0.381E-02	0.508E-01	0.207E-01
13.445	0.174E 01	0.565E 00	0.174E 01	0.276E-02	0.262E-02	0.353E-01	0.210E-01
13.545	0.172E 01	0.571E 00	0.173E 01	0.275E-02	0.515E-02	0.698E-01	0.212E-01
13.644	0.170E 01	0.577E 00	0.171E 01	0.272E-02	0.283E-02	0.386E-01	0.214E-01
13.741	0.169E 01	0.583E 00	0.168E 01	0.269E-02	-0.206E-02	-0.282E-01	0.216E-01
13.838	0.167E 01	0.589E 00	0.166E 01	0.267E-02	-0.559E-02	-0.774E-01	0.217E-01
14.028	0.164E 01	0.600E 00	0.164E 01	0.265E-02	0.332E-02	0.466E-01	0.223E-01
14.214	0.160E 01	0.612E 00	0.161E 01	0.262E-02	0.426E-02	0.606E-01	0.228E-01
14.395	0.158E 01	0.623E 00	0.158E 01	0.259E-02	0.306E-02	0.441E-01	0.232E-01
14.572	0.155E 01	0.634E 00	0.155E 01	0.255E-02	-0.249E-02	-0.363E-01	0.235E-01
14.744	0.152E 01	0.645E 00	0.153E 01	0.253E-02	0.486E-02	0.716E-01	0.240E-01
14.913	0.150E 01	0.656E 00	0.150E 01	0.249E-02	0.136E-02	0.203E-01	0.244E-01
15.076	0.148E 01	0.668E 00	0.148E 01	0.246E-02	0.158E-03	0.238E-02	0.248E-01

H_2O 200°C

S	F(S)	M(S)	J(S)	ERROR	I(S)	S*I(S)	ERROR
15.235	0.145E 01	0.679E 00	0.145E 01	0.243E-02	-0.150E-03	-0.229E-02	0.252E-01
15.389	0.143E 01	0.691E 00	0.143E 01	0.241E-02	-0.639E-03	-0.983E-02	0.256E-01
15.539	0.140E 01	0.702E 00	0.141E 01	0.238E-02	0.256E-02	0.398E-01	0.260E-01
15.684	0.139E 01	0.713E 00	0.139E 01	0.236E-02	0.479E-02	0.752E-01	0.264E-01
15.824	0.136E 01	0.723E 00	0.137E 01	0.233E-02	0.773E-02	0.122E 00	0.267E-01
15.959	0.135E 01	0.732E 00	0.135E 01	0.230E-02	0.224E-02	0.358E-01	0.268E-01

RADIAL DISTRIBUTION FUNCTIONS TO 10 A

H_2O 200°C

R	G(R)	R	G(R)	R	G(R)	R	G(R)
0.0	0.0	2.50	0.2652	5.00	0.9685	7.50	1.0014
0.05	1.1214	2.55	0.4817	5.05	0.9560	7.55	1.0101
0.10	0.7808	2.60	0.6373	5.10	0.9530	7.60	1.0186
0.15	0.3586	2.65	0.8309	5.15	0.9612	7.65	1.0222
0.20	0.0086	2.70	1.0515	5.20	0.9766	7.70	1.0183
0.25	-0.1523	2.75	1.2774	5.25	0.9919	7.75	1.0081
0.30	-0.0882	2.80	1.4806	5.30	1.0001	7.80	0.9957
0.35	0.1497	2.85	1.6342	5.35	0.9986	7.85	0.9863
0.40	0.4526	2.90	1.7210	5.40	0.9897	7.90	0.9831
0.45	0.7119	2.95	1.7386	5.45	0.9794	7.95	0.9865
0.50	0.8531	3.00	1.6998	5.50	0.9740	8.00	0.9932
0.55	0.8947	3.05	1.6266	5.55	0.9768	8.05	0.9988
0.60	0.8834	3.10	1.5419	5.60	0.9870	8.10	1.0001
0.65	0.9089	3.15	1.4624	5.65	1.0004	8.15	0.9967
0.70	1.0346	3.20	1.3951	5.70	1.0121	8.20	0.9909
0.75	1.2719	3.25	1.3377	5.75	1.0189	8.25	0.9868
0.80	1.5754	3.30	1.2841	5.80	1.0204	8.30	0.9875
0.85	1.8640	3.35	1.2287	5.85	1.0187	8.35	0.9933
0.90	2.0559	3.40	1.1700	5.90	1.0166	8.40	1.0018
0.95	2.1002	3.45	1.1107	5.95	1.0155	8.45	1.0089
1.00	1.9927	3.50	1.0559	6.00	1.0155	8.50	1.0110
1.05	1.7703	3.55	1.0107	6.05	1.0151	8.55	1.0069
1.10	1.4904	3.60	0.9779	6.10	1.0130	8.60	0.9988
1.15	1.2072	3.65	0.9590	6.15	1.0094	8.65	0.9904
1.20	0.9551	3.70	0.9542	6.20	1.0054	8.70	0.9857
1.25	0.7454	3.75	0.9630	6.25	1.0029	8.75	0.9867
1.30	0.5745	3.80	0.9838	6.30	1.0032	8.80	0.9928
1.35	0.4345	3.85	1.0129	6.35	1.0060	8.85	1.0010
1.40	0.3225	3.90	1.0433	6.40	1.0096	8.90	1.0076
1.45	0.2411	3.95	1.0662	6.45	1.0122	8.95	1.0103
1.50	0.1935	4.00	1.0733	6.50	1.0128	9.00	1.0087
1.55	0.1773	4.05	1.0603	6.55	1.0119	9.05	1.0045
1.60	0.1818	4.10	1.0296	6.60	1.0110	9.10	1.0003
1.65	0.1907	4.15	0.9897	6.65	1.0114	9.15	0.9981
1.70	0.1892	4.20	0.9526	6.70	1.0129	9.20	0.9987
1.75	0.1709	4.25	0.9284	6.75	1.0140	9.25	1.0009
1.80	0.1400	4.30	0.9212	6.80	1.0122	9.30	1.0031
1.85	0.1087	4.35	0.9278	6.85	1.0062	9.35	1.0037
1.90	0.0900	4.40	0.9395	6.90	0.9966	9.40	1.0022
1.95	0.0908	4.45	0.9471	6.95	0.9864	9.45	0.9993
2.00	0.1092	4.50	0.9455	7.00	0.9798	9.50	0.9964
2.05	0.1360	4.55	0.9363	7.05	0.9797	9.55	0.9948
2.10	0.1601	4.60	0.9262	7.10	0.9865	9.60	0.9949
2.15	0.1744	4.65	0.9232	7.15	0.9972	9.65	0.9965
2.20	0.1786	4.70	0.9320	7.20	1.0071	9.70	0.9986
2.25	0.1782	4.75	0.9509	7.25	1.0120	9.75	1.0002
2.30	0.1816	4.80	0.9727	7.30	1.0106	9.80	1.0007
2.35	0.1964	4.85	0.9885	7.35	1.0047	9.85	1.0000
2.40	0.2286	4.90	0.9921	7.40	0.9988	9.90	0.9987
2.45	0.2830	4.95	0.9834	7.45	0.9971	9.95	0.9977

5.2 Some Relevant Parameters for the Ice-I Model of Liquid Water, Obtained from Least-Squares Refinement Against the X-ray Data. Near-Neighbor Interactions P_1, P_2, and P_3 (Fig. 7) are Characterized by a Mean Distance r (Å) and RMS-Variation $\langle \Delta r^2 \rangle^{1/2}$ (Å). Fractional Occupancy of Network and Cavity Positions are f_1 and f_2, the Fraction of Molecules in the Respective Positions is w and (1-w).

		P_1		P_2		P_3				
		r	$\langle \Delta r^2 \rangle^{1/2}$	r	$\langle \Delta r^2 \rangle^{1/2}$	r	$\langle \Delta r^2 \rangle^{1/2}$	f_1	f_2	w
D_2O	4°C	2.90±0.01	0.20±0.01	2.78±0.01	0.09±0.01	2.93±0.01	0.78±0.05	1	0.42_5	0.82_4
H_2O	4°C	2.91±0.01	0.20±0.01	2.79±0.01	0.09±0.01	2.94±0.01	0.70±0.04	1	0.45_1	0.81_6
	20°C	2.94±0.01	0.18±0.01	2.78±0.01	0.08±0.01	2.96±0.01	0.53±0.04	1	0.51_3	0.79_6
	25°C	2.94±0.01	0.18±0.01	2.78±0.01	0.08±0.01	2.96±0.01	0.53±0.04	1	0.51_3	0.79_6
	50°C	2.96±0.01	0.16±0.01	2.74±0.01	0.05±0.01	2.98±0.01	0.45±0.03	1	0.49_1	0.80_3
	75°C	2.99±0.01	0.27±0.02	2.75±0.01	0.06±0.01	2.99±0.01	0.12±0.03	1	0.52_5	0.79_2
	100°C	3.02±0.01	0.22±0.02	2.76±0.01	0.12±0.01	3.02±0.01	0.43±0.06	0.9_9	0.5_5	0.7_8
	150°C	2.98±0.01	0.21±0.01	2.74±0.01	0.13±0.01	~3	*	0.8_7	0.6_2	0.7_4
	200°C	2.86±0.02	0.22±0.01	2.97±0.03	0.23±0.03	~3	*	0.7_9	0.5_7	0.7_3

*The variance in the P_3 distance is so large that the cavity molecules must be considered randomly located within van der Waals distance of the network molecules.

6. REFERENCES

1. H. H. Meyer, Ann. Physik, 5, 701 (1930).
2. G. W. Stewart, Phys. Rev., 37, 9 (1931).
3. E. Amaldi, Physik. Zeitschr., 32, 914 (1931).
4. S. Katzoff, J. Chem. Phys., 2, 841 (1934).
5. J. Morgan and B. E. Warren, J. Chem. Phys., 6, 666 (1938).
6. L. Simons, Soc. Sci. Fennica, Commentationes Phys. Math., 10, no. 9 (1939).
7. C. Finbak and H. Viervoll, Tidsskr. Kjemi, Bergvesen Met., 3, 36 (1943).
8. G. W. Brady and W. J. Romanow, J. Chem. Phys., 32, 306 (1960).
9. C. L. van Panthaleon van Eck, H. Mendel, and W. Boog, Disc. Faraday Soc., 24, 200 (1957); Proc. Roy Soc., A247, 472 (1958).
10. J. Heemskerk, Rec. Trav. Chim., 81, 904 (1962).
11. M. D. Danford and H. A. Levy, J. Am. Chem. Soc., 84, 3965 (1962).
12. A. H. Narten, M. D. Danford, and H. A. Levy, "X-Ray Diffraction Data on Liquid Water in the Temperature Range 4 - 200°C," ORNL-3997 (1966).
13. A. H. Narten, M. D. Danford, and H. A. Levy, Disc. Faraday Soc., 43, 97 (1967).
14. A. H. Narten and H. A. Levy, Science, 165, 447 (1969); Science, 167, 1520 (1970).

15. R. W. Hendricks, presented at the American Chemical Society Meeting, New York City, September 7 - 12 (1969); to be submitted to J. Chem. Phys.

16. L. B. Shaffer, Thesis, University of Wisconsin (1964).

17. P. Thomas, Zeitschr. Physik, 208, 338 (1968).

18. A. M. Levelut and A. Guinier, Bull. Soc. Franc. Mineral. Crystallogr., 40, 445 (1967).

19. N. J. Chonacky and W. H. Beeman, Acta Cryst., A25, 564 (1969).

20. W. Bol, J. Appl. Cryst., 1, 234 (1968).

21. H. A. Levy, M. D. Danford, and A. H. Narten, "Data Collection and Evaluation with an X-ray Diffractometer Designed for the Study of Liquid Structure," ORNL-3960 (1966).

22. A. Guinier, X-Ray Diffraction, W. H. Freeman Co., San Francisco, 1963, p. 346.

23. A. Rahman, J. Chem. Phys., 42, 3540 (1965).

24. Ref. 22, p. 46.

25. J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, Molecular Theory of Gases and Liquids, Wiley, New York, 1966, p. 122.

26. C. J. Pings and J. Waser, J. Chem. Phys., 48, 3016 (1968).

27. J. Waser and V. Schomaker, Rev. Mod. Phys., 25, 671 (1953).

28. W. Parish, Philips Tech. Rev., 17, 206 (1956).

29. D. T. Cromer and J. B. Mann, "X-Ray Scattering Factors Computed from Numerical Hartree-Fock Wave Functions," LA-3816 (1968); "Compton Scattering Factors for Spherically Symmetric Free Atoms," LA-3689 (1967); D. T. Cromer, Private Communication (Compton Scattering Factors for Hydrogen); R. F. Stewart, E. R. Davidson, and W. T. Simpson, J. Chem. Phys., 42, 3175 (1965) (Coherent Scattering Factors for Bonded Hydrogen).

30. D. I. Page, Disc. Faraday Soc., 43, 130 (1967).

31. W. S. Benedict, N. Gailar, and E. K. Plyler, J. Chem. Phys., 24, 1139 (1956).

32. S. Shibata and L. S. Bartell, J. Chem. Phys., 42, 1147 (1965).

33. C. J. Pings, in Physics of Simple Liquids, H. N. V. Temperley, J. S. Rowlinson, and G. S. Rushbrooke (Editors), North-Holland Publishing Co., Amsterdam, 1968, p. 405.

34. O. Y. Samoilov, Zh. Fiz, Khim., 20, 12 (1946).

35. A. H. Narten, J. Chem. Phys., 49, 1692 (1968).

36. S. LaPlaca and B. Post, Acta Cryst., 13, 503 (1960).

37. G. S. Kell, J. Chem. Eng. Data, 12, 66 (1967).

ORNL-4578
UC-4 — Chemistry

INTERNAL DISTRIBUTION

1. Biology Library
2-4. Central Research Library
5-6. ORNL — Y-12 Technical Library Document Reference Section
7-41. Laboratory Records Department
42. Laboratory Records, ORNL R.C.
43. C. F. Baes
44. G. E. Boyd
45. J. Braunstein
46. F. L. Culler
47. J. R. Einstein
48. R. W. Hendricks
49. R. F. Hibbs
50. K. A. Kraus
51. M. H. Lietzke
52. S. Lindenbaum
53. H. G. MacPherson
54. P. Mazur
55-104. A. H. Narten
105. A. S. Quist
106. R. M. Rush
107. M. J. Skinner
108. D. A. Sundberg
109. E. H. Taylor
110. F. Vaslow
111. A. M. Weinberg
112. P. D. Bartlett (consultant)
113. Gerhart Friedlander (consultant)
114. J. J. Katz (consultant)
115. F. A. Long (consultant)
116. J. E. Mayer (consultant)
117. G. Scatchard (consultant)
118. H. H. Sisler (consultant)

EXTERNAL DISTRIBUTION

119. H. S. Frank, Mellon Institute, 4400 Fifth Ave., Pittsburgh, Pennsylvania
120. O. Ya. Samoilov, N.S. Kurnakov Institute of General and Inorganic Chemistry, Academy of Sciences USSR, 31 Lenin Ave., Moscow, B-71, USSR
121. P. A. Egelstaff, Solid State Physics Division, AERE, Harwell, Berks., England
122. R. D. Larsen, Department of Chemistry, Illinois Institute of Technology, Chicago, Illinois
123. E. U. Franck, Department of Physical Chemistry, University of Karlsruhe, Karlsruhe, Germany
124. J. I. Padova, Soreq Nuclear Research Center, Yavne, Israel
125. Z. Bochynski, Department of Molecular Physics, University of Poznan, Poznan, Poland
126. C. J. Pings, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California
127. H. G. Hertz, Department of Physical Chemistry, University of Karlsruhe, Karlsruhe, Germany
128. A. J. Leadbetter, Chemistry Department, The University, Bristol, England
129. F. H. Stillinger, Bell Telephone Laboratories, Murray Hill, New Jersey
130. K. E. Larsson, The Royal Institute of Technology, Stockholm, Sweden
131. W. Luck, Central Laboratory, BASF, Ludwigshafen, Germany

132. G. Marongiu, University of Cagliari, Cagliari, Sardinia, Italy
133. A. Ben-Naim, Department of Inorganic and Analytical Chemistry, The Hebrew University, Jerusalem, Israel
134. H. Krebs, Department of Inorganic and Analytical Chemistry, Technical University of Stuttgart, Stuttgart, Germany
135. G. J. Safford, Sterling Forest Research Center, Union Carbide Corporation, Tuxedo, New York
136. M. Falk, Atlantic Regional Laboratory, National Research Council of Canada, Halifax, Nova Scotia, Canada
137. D. Evans, Research Laboratory, Corning Glass Works, Corning, New York
138. J. E. Enderby, Department of Physics, The University, Leicester, England
139. J. A. Swartout, Union Carbide Corporation, New York, N.Y.
140. Laboratory and University Division, AEC, ORO
141. Patent Office, AEC, ORO
142-331. Given distribution as shown in TID-4500 under Chemistry category (25 copies — CFSTI)