Molecular Form Factors and Photon Coherent Scattering Cross Sections of Water

L. R. M. Morin

15 Avenue Bosquet 75007 Paris, France

Tabulations are presented of molecular form factors $F(x)$, for values of $x = \sin(\theta/2)/\lambda$ from 0 to 1.25 Å^{-1}, for liquid water at eight temperatures between 4 °C and 200 °C and for the free water molecule. For liquid water, $x = 0$ to 1.25 Å^{-1}, the tabulated values are interpolated from experimental values of Narten and Levy (1971). For the free water molecule, $x = 0$ to 1.25 Å^{-1}, the tabulated values are interpolated from calculated values of Blum (1971). For $x = 1.25$ to 10^9 Å^{-1}, the independent atomic scattering hypothesis is assumed and the water molecular form factor $F(x)$ is calculated from the hydrogen and oxygen atomic form factors given by Hubbell and Overbo (1979). Tables of coherent scattering cross sections, obtained by numerical integration of the Thomson formula, weighted by $F^2(x)$, are presented for liquid water at eight temperatures between 4 °C and 200 °C and for the free water molecule, for photon energies 5 keV to 1 MeV.

Key words: coherent scattering; cross section; form factor; Rayleigh scattering; tabulation; water; x rays.

1. Introduction

Molecular form factors and photon coherent scattering cross sections of water are required in medical x-ray technology. Especially, their knowledge would help to understand artifacts due to single and multiple scattering in CT scanners.

Experiments on x-ray scattering by liquid water have been carried out at the Oak Ridge National Laboratory (most recent publication: Narten and Levy [1][1]) and by Hajdu et al. [2], for the purpose of studying the structure of liquid water. These authors do not give tabulations of water molecular form factors, but tabulations of water structure functions. Blum [3] has calculated molecular form factors for the free water molecule, with a method derived from Steele and Pecora [4] and a self-consistent-field molecular orbital calculation by Moccia [5].

For $x = \sin(\theta/2)/\lambda$ less than 1.25 Å^{-1}, tables of liquid water molecular form factors, derived from the structure functions of Narten and Levy [1], are presented here, together with a table of free water molecular form factors, interpolated from Blum [3]. For $x > 1.25$ Å^{-1}, a table of water molecular form factors is calculated from the hydrogen and oxygen relativistic Hartree-Fock form factors given by Hubbell and Overbo [6], using the independent atomic scattering hypothesis. A table of integrated coherent (Rayleigh) scattering cross section values, computed for photon energies 5 keV to 1 MeV using the above form factors, is also presented.

[1]Figures in brackets indicate literature references at the end of this paper.

2. Physical Constants, Notation, and Units

b	barn $= 10^{-28}$ m^2
r_e	classical electron radius $= 2.8179380 \cdot 10^{-15}$ m
E	photon energy
λ	photon wavelength
θ	angle between the photon direction of travel prior to and following a scattering interaction
x	$= \sin(\theta/2)/\lambda$
$d\Omega$	differential solid angle in steradian $= 2\pi \sin\theta \, d\theta$
$d\sigma_T(\theta)/d\Omega$	differential Thomson scattering cross section per electron $= \dfrac{r_e^2}{2}(1 + \cos^2\theta)$
$F_H(x)$	Hydrogen atomic form factor
$F_O(x)$	Oxygen atomic form factor
$F_{at}^W(x)$	water molecular form factor, calculated with the independent atomic scattering approximation (table 2)

$$F_{at}^W(x) = \left[2[F_H(x)]^2 + [F_O(x)]^2 \right]^{1/2} \tag{1}$$

$F_{mol}^W(x)$	molecular form factor for free water molecule (table 1)
$F_{liq}^W(x)$	molecular form factor for liquid water (table 1)
σ_{mol}	coherent (Rayleigh) scattering cross section per free water molecule (table 3)

$$= \int_{\theta=0}^{\theta=\pi} d\sigma_T(\theta) [F_{mol}^W(x)]^2 \tag{2}$$

σ_{liq}	coherent (Rayleigh) scattering cross section per liquid water molecule (table 3)

$$= \int_{\theta=0}^{\theta=\pi} d\sigma_T(\theta) [F_{liq}^W(x)]^2 \tag{3}$$

3. Composition of the *F(x)* Tables

3.1. Free Water Molecule

For $x = 0$ to 1.25 Å^{-1}, the values of $F^W_{mol}(x)$ (table 1) have been calculated by Lagrangian interpolation from calculated values of Blum [3].

3.2. Liquid Water

For $x = 0$ to 1.25 Å^{-1}, the values of $F^W_{liq}(x)$ at 4 °C, 20 °C, 25 °C, 50 °C, 75 °C, 100 °C, 150 °C, 200 °C (table 1) have been derived from experimental values of Narten and Levy [1]. The pressure is supposed to be atmospheric pressure at temperatures below 100 °C and equal to the vapor pressure above 100 °C.

3.3. Independent Atomic Scattering Hypothesis

In this hypothesis, each atom of the water molecule is supposed to radiate by itself independently from the other atoms. $F(x)$ in this hypothesis can be calculated from the hydrogen and oxygen atomic form factors, using eq (1).

This hypothesis is valid for $x > 1.25$ Å^{-1}. When x is small, Rayleigh scattering includes outer electrons which are involved in the water molecule. When x gets larger, Rayleigh scattering includes in practice only inner electrons of the oxygen atom. For $x > 1.25$ Å^{-1}, the oxygen atomic form factor is small as compared with 8. This ensures that the contribution of the outer electrons of the water molecule is negligible and that the independent atomic scattering hypothesis is valid.

The molecular form factors $F^W_{at}(x)$ have been calculated within this hypothesis, from the oxygen and hydrogen relativistic atomic form factors given by Hubbell and Overbo [6], and using eq (1). For $x > 1.25$ Å^{-1}, $F^W_{at}(x)$ is equal to the oxygen atomic form factor $F_O(x)$, to the three figures accuracy given here. Table 2 contains values of $F^W_{at}(x)$ for $x = 1.25$ to 10^9 Å^{-1}. The values of $F^W_{at}(x)$ for $x = 0$ to 1.25 Å^{-1} are also listed in table 1 for comparison with $F^W_{mol}(x)$ and $F^W_{liq}(x)$. For 1 Å$^{-1} < x < 1.25$ Å^{-1}, $F^W_{liq}(x)$ and $F^W_{at}(x)$ differ by less than 1%, but this is the result of the normalization process used by Narten [7], which requires: $F^W_{liq}(x) \simeq F^W_{at}(x)$ at large x.

The $F^W_{at}(x)$ values are theoretical values which provide an approximation for $F^W_{liq}(x)$ and $F^W_{mol}(x)$ in the region where there is no available data, i.e., for $x > 1.25$ Å^{-1}. Attention is called on the fact that for $x > 4$ Å^{-1}, the form factor approximation fails to decrease as rapidly as predicted by more accurate theory by Kissel et al. [8] (see sec. 3.4). To stress that point, values of $F^W_{at}(x)$ for $x > 4$ Å^{-1} have been put into parenthesis in table 2.

3.4. Validity of Form Factor Approximation

Kissel et al. [8] have calculated Rayleigh scattering, describing the atom as N non-interacting bound electrons in a relativistic self consistent central potential. They have found that for $x > 4$ Å^{-1}, the form factor approximation fails to decrease as rapidly as their numerical predictions. To stress that point, values of $F^W_{at}(x)$ for $x > 4$ Å^{-1} have been put into parenthesis in table 2.

3.5. Choice of the *F(x)* Values

For $x = 0$ to 1.25 Å^{-1} and for liquid water, $F(x)$ can be taken from the experimental values $F^W_{liq}(x)$ of table 1. For $x = 0$ to 1.25 Å^{-1} and for the free water molecule or for the water molecule in the gas, $F(x)$ can be taken from the theoretical values $F^W_{mol}(x)$ of table 1. Differences between $F^W_{mol}(x)$ and $F^W_{liq}(x)$ are due to the intermolecular interferences effects which take place in liquid water (James [9]). The importance of the differences between $F^W_{mol}(0)$ and $F^W_{liq}(0)$ comes from that scattering intensity by fluids at zero angle is related to isothermal compressibility (Guinier [10]).

For 1.25 Å$^{-1} < x < 4$ Å^{-1}, $F(x)$ can be taken from theoretical values $F^W_{at}(x)$ of table 2, which gives the form factor of water in the independent atomic scattering approximation. For $x > 4$ Å^{-1}, $F(x)$ can be taken from table 2, bearing in mind that, at large x, form factor approximation fails to decrease as rapidly as predicted by Kissel et al. [8] (see sec. 3.4).

4. Total Cross Sections for Coherent (Rayleigh) Scattering of Photons by Water

Values of integrated coherent scattering cross sections σ_{mol}, σ_{liq}, obtained using eq (2) and (3), respectively, and the $F^W_{mol}(x)$, $F^W_{liq}(x)$ and $F^W_{at}(x)$ values of tables 1 and 2, are presented in table 3 over the photon energy range 5 keV to 1 MeV. For $x > 1.25$ Å^{-1}, the independent atomic scattering value $F^W_{at}(x)$ has been taken as an approximation for $F^W_{mol}(x)$ and $F^W_{liq}(x)$. The numerical integration procedure used the trapezoid rule, with the integration variable taken as $(1 - \cos\theta)$ and a mesh of 1001 logarithmically spaced points (1000 intervals) over the range $10^{-12} \leqslant (1 - \cos\theta) \leqslant 2$. Values of $F^W_{mol}(x)$ and $F^W_{liq}(x)$ at the integration mesh points were obtained by Lagrangian interpolation from values listed in table 1. Values of $F^W_{at}(x)$ at the integration mesh points were obtained by log-log linear interpolation from values listed in table 2.

For $E < 50$ keV, the integration extends only to values of $x < 4$ Å^{-1} and the inaccuracy of form factor approximation at large x has no incidence upon the integrated cross sections. For $E > 50$ keV, the integration extends to values of $x > 4$ Å^{-1}, but the contribution of these values to the integrated cross section is less than 2%. As form factor approximation overestimates Rayleigh scattering at large x (see sec. 3.4), the incidence of such inaccuracy upon the integrated cross sections is less than 2%. To stress that point, values of σ for $E > 50$ keV have been put into parenthesis in table 3.

For the free water molecule or for the water molecule in the gas, the cross sections can be taken from the σ_{mol} values given in the column "molecular water" of table 3. For liquid water, the cross sections can be taken from the σ_{liq} values listed in the columns "liquid water" of table 3. For liquid water, $E \leqslant 15$ keV, the integration uses only values of $x < 1.25$ Å^{-1} and so the σ_{liq} values are calculated only from experimental results of Narten and Levy [1]. For liquid water, $E > 15$ keV, the integration extends to values of $x > 1.25$ Å^{-1} and so it uses both experimental results of Narten and Levy [1] and theoretical results of Hubbell and Overbo [6].

The differences between the form factors $F^W_{mol}(x)$ and $F^W_{liq}(x)$ (sec. 3.5) have repercussions upon the integrated cross

Table 1. WATER MOLECULAR FORM FACTORS F(X) a

X SIN(THETA/2)/LAMBDA	LIQUID WATER 4°C	LIQUID WATER 20°C	LIQUID WATER 25°C	LIQUID WATER 50°C	LIQUID WATER 75°C	LIQUID WATER 100°C	LIQUID WATER 150°C	LIQUID WATER 200°C	MOLECULAR WATER	INDEPENDENT ATOMIC SCATTERING
.000	2.51	2.49	2.49	2.55	2.66	2.85	3.33	3.91	10.00	8.12
.005	2.53	2.49	2.49	2.55	2.68	2.85	3.34	3.91	10.00	8.12
.010	2.53	2.48	2.49	2.55	2.68	2.84	3.35	3.91	9.99	8.12
.015	2.52	2.49	2.49	2.55	2.68	2.84	3.38	3.93	9.97	8.10
.020	2.52	2.52	2.50	2.56	2.69	2.85	3.41	3.94	9.95	8.09
.025	2.53	2.51	2.49	2.55	2.70	2.84	3.41	3.94	9.91	8.07
.030	2.53	2.52	2.50	2.55	2.70	2.86	3.41	3.95	9.87	8.05
.035	2.54	2.52	2.51	2.56	2.70	2.87	3.43	3.96	9.83	8.01
.040	2.54	2.52	2.51	2.57	2.71	2.87	3.45	3.98	9.78	7.99
.045	2.56	2.52	2.55	2.60	2.74	2.89	3.47	4.02	9.72	7.95
.050	2.60	2.54	2.58	2.68	2.79	2.92	3.51	4.06	9.65	7.91
.055	2.65	2.56	2.66	2.78	2.87	2.98	3.56	4.11	9.58	7.86
.060	2.71	2.58	2.74	2.93	2.95	3.05	3.61	4.17	9.51	7.82
.065	2.79	2.60	2.82	3.03	3.04	3.13	3.67	4.24	9.42	7.77
.070	2.89	2.62	2.93	3.12	3.15	3.24	3.75	4.31	9.34	7.72
.075	3.03	2.64	3.04	3.18	3.28	3.40	3.86	4.37	9.25	7.66
.080	3.20	2.74	3.14	3.23	3.43	3.58	3.98	4.42	9.15	7.60
.085	3.37	2.86	3.24	3.31	3.58	3.79	4.10	4.47	9.05	7.54
.090	3.52	2.99	3.38	3.42	3.72	3.98	4.21	4.53	8.95	7.47
.095	3.68	3.17	3.58	3.55	3.85	4.14	4.32	4.60	8.84	7.40
.100	3.87	3.39	3.83	3.70	4.01	4.29	4.47	4.71	8.72	7.34
.105	4.13	3.67	4.11	3.92	4.24	4.48	4.65	4.86	8.61	7.26
.110	4.45	4.01	4.40	4.24	4.53	4.72	4.85	5.05	8.49	7.19
.115	4.82	4.38	4.74	4.64	4.84	5.00	5.09	5.28	8.37	7.11
.120	5.22	4.80	5.13	5.11	5.17	5.30	5.37	5.54	8.25	7.03
.125	5.67	5.27	5.60	5.59	5.53	5.63	5.64	5.82	8.12	6.95
.130	6.17	5.78	6.11	6.08	5.93	5.93	5.94	6.12	8.00	6.87
.135	6.68	6.31	6.63	6.56	6.38	6.33	6.25	6.41	7.87	6.79
.140	7.14	6.82	7.10	7.05	6.82	6.68	6.57	6.70	7.74	6.71
.145	7.50	7.25	7.48	7.48	7.22	7.03	6.82	6.96	7.61	6.62
.150	7.74	7.58	7.74	7.82	7.52	7.30	7.06	7.19	7.48	6.54
.155	7.83	7.76	7.88	8.03	7.72	7.48	7.32	7.39	7.35	6.45
.160	7.78	7.82	7.89	8.10	7.81	7.58	7.59	7.54	7.22	6.36
.165	7.62	7.75	7.80	8.06	7.82	7.63	7.77	7.65	7.09	6.27
.170	7.39	7.59	7.64	7.94	7.77	7.62	7.77	7.71	6.96	6.19
.175	7.15	7.38	7.43	7.77	7.66	7.56	7.68	7.72	6.83	6.10
.180	6.94	7.17	7.21	7.57	7.52	7.44	7.59	7.69	6.70	6.01
.185	6.77	6.98	7.00	7.37	7.36	7.27	7.49	7.61	6.58	5.92
.190	6.63	6.83	6.82	7.18	7.18	7.08	7.33	7.50	6.45	5.84
.195	6.51	6.70	6.68	7.02	7.02	6.90	7.14	7.34	6.33	5.75
.200	6.42	6.60	6.59	6.89	6.88	6.76	6.99	7.16	6.20	5.66
.205	6.38	6.53	6.54	6.79	6.76	6.65	6.84	6.95	6.08	5.57
.210	6.37	6.49	6.51	6.70	6.65	6.54	6.64	6.73	5.96	5.49
.215	6.39	6.48	6.49	6.61	6.54	6.41	6.38	6.49	5.84	5.40
.220	6.40	6.46	6.46	6.51	6.41	6.31	6.15	6.25	5.73	5.32
.225	6.39	6.44	6.39	6.39	6.24	6.17	5.98	6.00	5.61	5.24
.230	6.34	6.36	6.27	6.22	6.05	6.11	5.81	5.76	5.50	5.15
.235	6.23	6.23	6.10	6.00	5.82	5.82	5.58	5.53	5.39	5.07
.240	6.06	6.03	5.87	5.73	5.57	5.59	5.38	5.31	5.28	4.99
.245	5.80	5.76	5.61	5.43	5.30	5.33	5.22	5.10	5.18	4.91

Table 1. WATER MOLECULAR FORM FACTORS F(X) ^a --Continued

X SIN(THETA/2)/LAMBDA	LIQUID WATER 4 °C	LIQUID WATER 20 °C	LIQUID WATER 25 °C	LIQUID WATER 50 °C	LIQUID WATER 75 °C	LIQUID WATER 100 °C	LIQUID WATER 150 °C	LIQUID WATER 200 °C	MOLECULAR WATER	INDEPENDENT ATOMIC SCATTERING
.250	5.49	5.46	5.32	5.12	5.05	5.07	5.06	4.91	5.07	4.83
.255	5.15	5.14	5.01	4.82	4.77	4.83	4.84	4.73	4.97	4.75
.260	4.82	4.82	4.71	4.54	4.54	4.52	4.57	4.57	4.87	4.68
.265	4.53	4.54	4.44	4.28	4.34	4.44	4.38	4.43	4.77	4.60
.270	4.30	4.30	4.20	4.08	4.18	4.29	4.27	4.30	4.68	4.52
.275	4.11	4.10	4.01	3.92	4.05	4.15	4.20	4.19	4.59	4.45
.280	3.95	3.93	3.87	3.84	3.89	4.03	4.09	4.09	4.50	4.38
.285	3.83	3.81	3.76	3.74	3.85	3.94	4.03	4.01	4.41	4.31
.290	3.74	3.72	3.70	3.69	3.85	3.87	3.97	3.94	4.32	4.24
.295	3.68	3.66	3.67	3.65	3.79	3.83	3.92	3.88	4.24	4.17
.300	3.64	3.62	3.65	3.63	3.76	3.79	3.86	3.83	4.16	4.10
.305	3.61	3.60	3.65	3.61	3.73	3.76	3.81	3.80	4.08	4.04
.310	3.60	3.59	3.64	3.60	3.71	3.73	3.79	3.76	4.00	3.97
.315	3.60	3.59	3.63	3.59	3.70	3.71	3.78	3.74	3.93	3.91
.320	3.59	3.59	3.63	3.60	3.68	3.71	3.77	3.72	3.86	3.85
.325	3.60	3.59	3.63	3.60	3.67	3.71	3.76	3.70	3.79	3.78
.330	3.60	3.59	3.63	3.61	3.65	3.69	3.71	3.68	3.72	3.72
.335	3.59	3.59	3.63	3.60	3.64	3.67	3.68	3.66	3.65	3.67
.340	3.58	3.59	3.63	3.60	3.62	3.64	3.64	3.64	3.59	3.61
.345	3.57	3.58	3.61	3.59	3.60	3.61	3.60	3.61	3.52	3.55
.350	3.55	3.57	3.59	3.57	3.57	3.59	3.57	3.58	3.46	3.50
.355	3.53	3.54	3.56	3.55	3.53	3.55	3.53	3.54	3.40	3.44
.360	3.50	3.51	3.52	3.53	3.50	3.51	3.46	3.50	3.35	3.39
.365	3.47	3.48	3.48	3.49	3.46	3.46	3.35	3.45	3.31	3.34
.370	3.43	3.44	3.44	3.44	3.42	3.40	3.32	3.40	3.24	3.29
.375	3.38	3.40	3.39	3.39	3.38	3.35	3.27	3.35	3.18	3.24
.380	3.32	3.35	3.34	3.35	3.32	3.30	3.21	3.29	3.13	3.19
.385	3.27	3.30	3.29	3.29	3.26	3.24	3.15	3.23	3.08	3.15
.390	3.22	3.24	3.23	3.24	3.20	3.18	3.10	3.17	3.04	3.10
.395	3.17	3.18	3.17	3.17	3.13	3.11	3.10	3.10	2.99	3.06
.400	3.11	3.11	3.10	3.10	3.07	3.05	3.04	3.04	2.95	3.01
.405	3.05	3.05	3.03	3.03	3.01	2.99	2.98	2.98	2.90	2.97
.410	2.99	2.98	2.96	2.97	2.95	2.94	2.91	2.91	2.86	2.93
.415	2.92	2.91	2.89	2.91	2.89	2.88	2.85	2.85	2.82	2.89
.420	2.85	2.84	2.83	2.85	2.84	2.82	2.79	2.79	2.79	2.85
.425	2.79	2.77	2.77	2.78	2.77	2.75	2.73	2.73	2.74	2.81
.430	2.72	2.70	2.70	2.72	2.70	2.68	2.68	2.68	2.70	2.77
.435	2.65	2.64	2.64	2.66	2.64	2.63	2.63	2.63	2.67	2.74
.440	2.59	2.58	2.58	2.60	2.59	2.59	2.58	2.58	2.63	2.70
.445	2.54	2.53	2.53	2.55	2.54	2.55	2.52	2.53	2.60	2.67
.450	2.49	2.47	2.47	2.50	2.50	2.50	2.49	2.49	2.56	2.63
.455	2.44	2.43	2.42	2.45	2.45	2.46	2.45	2.45	2.53	2.60
.460	2.40	2.38	2.38	2.41	2.41	2.41	2.42	2.42	2.50	2.57
.465	2.35	2.34	2.34	2.38	2.38	2.38	2.39	2.39	2.47	2.54
.470	2.32	2.30	2.31	2.35	2.35	2.35	2.37	2.37	2.44	2.51
.475	2.29	2.28	2.29	2.32	2.32	2.34	2.34	2.34	2.42	2.48
.480	2.27	2.25	2.27	2.30	2.30	2.32	2.32	2.33	2.39	2.45
.485	2.25	2.24	2.25	2.26	2.28	2.31	2.31	2.31	2.36	2.42
.490	2.23	2.23	2.24	2.22	2.26	2.30	2.29	2.29	2.34	2.39
.495	2.22	2.22	2.23	2.21	2.25	2.29	2.27	2.28	2.31	2.37

Table 1. WATER MOLECULAR FORM FACTORS F(X) a—Continued

X = SIN(THETA/2)/LAMBDA	LIQUID WATER 4°C	LIQUID WATER 20°C	LIQUID WATER 25°C	LIQUID WATER 50°C	LIQUID WATER 75°C	LIQUID WATER 100°C	LIQUID WATER 150°C	LIQUID WATER 200°C	MOLECULAR WATER	INDEPENDENT ATOMIC SCATTERING
.500	2.21	2.21	2.22	2.20	2.24	2.28	2.25	2.27	2.29	2.34
.505	2.21	2.21	2.22	2.19	2.23	2.27	2.25	2.26	2.26	2.32
.510	2.20	2.20	2.21	2.19	2.21	2.25	2.24	2.25	2.24	2.29
.515	2.19	2.20	2.20	2.19	2.20	2.22	2.24	2.24	2.22	2.27
.520	2.18	2.20	2.19	2.19	2.19	2.19	2.20	2.22	2.20	2.25
.525	2.18	2.19	2.19	2.18	2.18	2.17	2.16	2.21	2.17	2.22
.530	2.18	2.19	2.18	2.17	2.17	2.16	2.16	2.19	2.15	2.20
.535	2.18	2.18	2.18	2.17	2.17	2.15	2.16	2.17	2.13	2.18
.540	2.17	2.17	2.17	2.17	2.16	2.14	2.16	2.15	2.12	2.16
.545	2.16	2.16	2.16	2.16	2.15	2.12	2.15	2.13	2.10	2.14
.550	2.15	2.15	2.15	2.15	2.14	2.11	2.13	2.11	2.08	2.12
.555	2.13	2.14	2.14	2.13	2.12	2.09	2.11	2.09	2.06	2.10
.560	2.11	2.12	2.12	2.11	2.10	2.08	2.10	2.07	2.04	2.08
.565	2.10	2.11	2.10	2.10	2.08	2.07	2.08	2.05	2.03	2.06
.570	2.08	2.09	2.08	2.08	2.06	2.05	2.05	2.03	2.01	2.05
.575	2.06	2.07	2.06	2.06	2.04	2.03	2.02	2.01	2.00	2.03
.580	2.04	2.04	2.04	2.04	2.02	2.01	1.99	1.99	1.98	2.01
.585	2.02	2.01	2.02	2.01	2.00	1.99	1.98	1.97	1.97	1.99
.590	2.00	1.99	1.99	1.99	1.98	1.97	1.97	1.95	1.95	1.98
.595	1.97	1.96	1.97	1.97	1.96	1.95	1.95	1.93	1.94	1.96
.600	1.95	1.94	1.94	1.95	1.93	1.93	1.92	1.92	1.92	1.95
.605	1.92	1.91	1.92	1.93	1.91	1.92	1.90	1.90	1.91	1.93
.610	1.90	1.89	1.89	1.90	1.89	1.90	1.88	1.89	1.90	1.92
.615	1.88	1.87	1.87	1.88	1.88	1.88	1.88	1.87	1.88	1.91
.620	1.86	1.85	1.85	1.86	1.86	1.86	1.87	1.86	1.87	1.89
.625	1.84	1.83	1.83	1.84	1.84	1.85	1.85	1.85	1.86	1.88
.630	1.82	1.81	1.81	1.82	1.82	1.83	1.83	1.84	1.85	1.87
.635	1.80	1.80	1.80	1.80	1.81	1.82	1.82	1.82	1.84	1.85
.640	1.79	1.78	1.78	1.79	1.79	1.81	1.81	1.81	1.83	1.84
.645	1.77	1.77	1.77	1.77	1.78	1.79	1.80	1.80	1.81	1.83
.650	1.76	1.76	1.75	1.76	1.77	1.78	1.78	1.80	1.80	1.82
.655	1.75	1.75	1.74	1.75	1.76	1.77	1.78	1.79	1.79	1.81
.660	1.74	1.74	1.74	1.75	1.75	1.76	1.78	1.78	1.78	1.79
.665	1.73	1.74	1.73	1.74	1.74	1.76	1.77	1.77	1.77	1.78
.670	1.73	1.73	1.73	1.73	1.73	1.75	1.76	1.76	1.76	1.77
.675	1.72	1.73	1.72	1.73	1.72	1.74	1.74	1.75	1.75	1.76
.680	1.72	1.72	1.72	1.72	1.72	1.73	1.74	1.74	1.74	1.75
.685	1.71	1.72	1.72	1.71	1.72	1.72	1.73	1.74	1.73	1.74
.690	1.71	1.71	1.72	1.71	1.71	1.72	1.72	1.73	1.72	1.73
.695	1.71	1.71	1.72	1.71	1.71	1.71	1.72	1.72	1.72	1.72
.700	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71
.705	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.70	1.71
.710	1.70	1.71	1.71	1.70	1.70	1.70	1.70	1.70	1.70	1.70
.715	1.70	1.70	1.70	1.70	1.70	1.69	1.69	1.69	1.69	1.69
.720	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.68	1.68	1.68
.725	1.69	1.69	1.69	1.69	1.69	1.68	1.68	1.68	1.67	1.67
.730	1.69	1.69	1.69	1.68	1.68	1.68	1.66	1.67	1.66	1.67
.735	1.68	1.68	1.68	1.68	1.68	1.57	1.66	1.66	1.66	1.66
.740	1.67	1.68	1.67	1.67	1.67	1.66	1.66	1.65	1.65	1.65
.745	1.67	1.67	1.67	1.67	1.66	1.66	1.65	1.65	1.64	1.64

Table 1. WATER MOLECULAR FORM FACTORS F(X) a —Continued

X SIN(THETA/2)/LAMBDA	LIQUID WATER 4°C	LIQUID WATER 20°C	LIQUID WATER 25°C	LIQUID WATER 50°C	LIQUID WATER 75°C	LIQUID WATER 100°C	LIQUID WATER 150°C	LIQUID WATER 200°C	MOLECULAR WATER	INDEPENDENT ATOMIC SCATTERING
.750	1.66	1.66	1.66	1.66	1.65	1.65	1.64	1.64	1.63	1.64
.755	1.65	1.65	1.65	1.65	1.65	1.64	1.64	1.63	1.63	1.63
.760	1.64	1.64	1.64	1.64	1.64	1.63	1.63	1.63	1.62	1.62
.765	1.63	1.63	1.63	1.62	1.63	1.62	1.62	1.62	1.61	1.62
.770	1.62	1.62	1.62	1.61	1.62	1.61	1.60	1.61	1.61	1.61
.775	1.61	1.61	1.61	1.60	1.61	1.61	1.59	1.60	1.60	1.60
.780	1.60	1.60	1.60	1.60	1.60	1.60	1.59	1.60	1.59	1.59
.785	1.59	1.59	1.59	1.59	1.59	1.59	1.58	1.59	1.59	1.59
.790	1.58	1.58	1.58	1.58	1.58	1.58	1.58	1.58	1.58	1.58
.795	1.57	1.57	1.57	1.57	1.57	1.57	1.57	1.57	1.58	1.57
.800	1.56	1.56	1.56	1.56	1.56	1.57	1.57	1.57	1.57	1.57
.810	1.54	1.54	1.55	1.54	1.55	1.55	1.55	1.56	1.56	1.56
.820	1.53	1.53	1.53	1.53	1.54	1.54	1.55	1.54	1.55	1.55
.830	1.52	1.52	1.51	1.52	1.53	1.53	1.53	1.53	1.54	1.53
.840	1.51	1.51	1.51	1.51	1.51	1.52	1.52	1.51	1.53	1.52
.850	1.50	1.51	1.50	1.51	1.51	1.51	1.52	1.51	1.52	1.51
.860	1.49	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.51	1.50
.870	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.50	1.49
.880	1.48	1.49	1.48	1.48	1.49	1.48	1.48	1.49	1.49	1.48
.890	1.48	1.48	1.48	1.48	1.48	1.48	1.47	1.48	1.48	1.47
.900	1.47	1.47	1.47	1.47	1.47	1.47	1.47	1.47	1.47	1.46
.910	1.47	1.47	1.46	1.46	1.46	1.46	1.46	1.46	1.46	1.45
.920	1.46	1.46	1.45	1.46	1.45	1.45	1.44	1.45	1.45	1.44
.930	1.45	1.45	1.44	1.45	1.45	1.44	1.44	1.44	1.44	1.44
.940	1.44	1.44	1.44	1.43	1.44	1.44	1.43	1.43	1.43	1.43
.950	1.43	1.43	1.42	1.42	1.43	1.42	1.42	1.42	1.42	1.42
.960	1.42	1.42	1.41	1.42	1.42	1.42	1.42	1.41	1.42	1.41
.970	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.41	1.40
.980	1.40	1.40	1.40	1.40	1.40	1.40	1.40	1.40	1.40	1.39
.990	1.38	1.38	1.38	1.39	1.39	1.39	1.39	1.38	1.39	1.39
1.000	1.37	1.37	1.37	1.38	1.38	1.38	1.38	1.38	1.38	1.38
1.020	1.35	1.35	1.36	1.36	1.36	1.36	1.36	1.36	1.36	1.36
1.040	1.34	1.34	1.34	1.34	1.34	1.34	1.35	1.35	1.34	1.34
1.060	1.33	1.33	1.33	1.33	1.33	1.33	1.33	1.33	1.33	1.33
1.080	1.32	1.32	1.32	1.31	1.31	1.31	1.31	1.32	1.31	1.31
1.100	1.30	1.30	1.30	1.30	1.30	1.30	1.30	1.29	1.30	1.30
1.120	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28
1.140	1.26	1.26	1.27	1.27	1.26	1.26	1.26	1.26	1.26	1.27
1.160	1.25	1.25	1.25	1.25	1.25	1.25	1.25	1.25	1.25	1.25
1.180	1.23	1.23	1.23	1.24	1.24	1.23	1.23	1.23	1.23	1.24
1.200	1.22	1.22	1.22	1.22	1.22	1.22	1.22	1.22	1.22	1.22
1.220	1.20	1.20	1.20	1.20	1.20	1.20	1.20	1.20	1.20	1.20
1.240	1.19	1.19	1.19	1.18	1.18	1.19	1.19	1.19	1.19	1.19
1.250	1.18	1.18	1.18	1.18	1.18	1.18	1.18	1.18	1.18	1.18

a LIQUID WATER = EXPERIMENTAL VALUES
MOLECULAR WATER = THEORICAL VALUES
INDEPENDENT ATOMIC SCATTERING = THEORICAL VALUES

Table 2. WATER MOLECULAR FORM FACTOR F(X) [a]
INDEPENDENT ATOMIC SCATTERING

X SIN(THETA/2)/LAMBDA	F(X)	X SIN(THETA/2)/LAMBDA	F(X)
1.25	1.18	6.2	(.330E-01)
1.3	1.15	6.6	(.265E-01)
1.4	1.07	7.0	(.216E-01)
1.5	.997	7.4	(.177E-01)
1.6	.926	8.0	(.133E-01)
1.7	.857	9.0	(.863E-02)
1.8	.792	10.	(.582E-02)
1.9	.731	11.	(.406E-02)
2.0	.674	12.	(.291E-02)
2.2	.570	14.	(.161E-02)
2.4	.482	16.	(.960E-03)
2.5	.443	18.	(.607E-03)
2.6	.407	20.	(.402E-03)
2.8	.345	22.	(.277E-03)
3.0	.293	25.	(.167E-03)
3.3	.230	28.	(.107E-03)
3.5	.196	31.	(.718E-04)
3.6	.182	35.	(.445E-04)
3.9	.145	40.	(.263E-04)
4.0	.135	45.	(.165E-04)
4.2	(.117)	50.	(.109E-04)
4.6	(.883E-01)	70.	(.292E-05)
5.0	(.678E-01)	.10E+03	(.724E-06)
5.4	(.527E-01)	.10E+04	(.139E-09)
5.5	(.496E-01)	.10E+07	(.751E-19)
5.8	(.415E-01)	.10E+10	(.768E-28)
6.0	(.369E-01)		

[a] THEORICAL

sections σ_{mol} and σ_{liq}. As the $F(x)$ differences are mostly important for low x, the $\sigma(E)$ differences are mostly important for low photon energies. Both the $F(x)$ and $\sigma(E)$ differences are due to the intermolecular interferences effects which take place in liquid water.

5. Discussion

Values of $F^W_{mol}(x)$ have also been calculated by Tavard [11]. Hajdu [12] has provided an analytic fit for the values of Tavard [11], for $x = 0$ to 1.2 Å^{-1}. Discrepancies between the $F^W_{mol}(x)$ values of Blum [3] and those of Tavard-Hajdu are less than .3% for $x = 0$ to 1.2 Å^{-1}. Discrepancies between the integrated values of σ_{mol} are less than .3%.

Liquid water molecular form factors $F^W_{liq}(x)$ at 4 °C, 25 °C, 50 °C and for $x = 0$ to .8 Å^{-1}, can also be derived from Hajdu et al. [2]. Discrepancies between the values of $F^W_{liq}(x)$, $x = 0$ to .8 Å^{-1}, derived from Narten and Levy [1] and from Hajdu et al. [2] are less than 10%. Discrepancies between the integrated values of σ_{liq} are less than 8.3%.

For $x > 4$ Å^{-1}, form factor approximation fails to decrease as rapidly as predicted by Kissel et al. [8]. However the effect upon integrated cross sections is zero for $E < 50$ keV and is less than 2% for $E > 50$ keV.

Acknowledgments

Table 3. WATER COHERENT SCATTERING CROSS-SECTIONS, BARNS/MOLECULE [a,b,c]

PHOTON ENERGY KEV	LIQUID WATER 4°C	LIQUID WATER 20°C	LIQUID WATER 25°C	LIQUID WATER 50°C	LIQUID WATER 75°C	LIQUID WATER 100°C	LIQUID WATER 150°C	LIQUID WATER 200°C	MOLECULAR WATER
5.0	14.8	14.7	14.9	15.2	15.0	14.9	15.2	15.6	20.5
6.0	12.1	12.0	12.2	12.4	12.2	12.2	12.3	12.6	16.2
8.0	8.59	8.53	8.64	8.76	8.68	8.63	8.73	8.90	10.9
10.	6.48	6.44	6.51	6.59	6.54	6.50	6.57	6.68	7.97
15.	3.81	3.79	3.82	3.86	3.83	3.82	3.85	3.90	4.48
20.	2.55	2.54	2.56	2.58	2.56	2.55	2.57	2.60	2.93
30.	1.36	1.35	1.36	1.37	1.36	1.36	1.37	1.38	1.53
40.	.834	.832	.836	.841	.838	.836	.840	.847	.929
50.	(.563)	(.561)	(.564)	(.567)	(.565)	(.564)	(.567)	(.571)	(.623)
60.	(.405)	(.404)	(.406)	(.408)	(.407)	(.406)	(.408)	(.411)	(.447)
80.	(.238)	(.237)	(.238)	(.240)	(.239)	(.238)	(.239)	(.241)	(.261)
.10E+03	(.156)	(.156)	(.156)	(.157)	(.157)	(.156)	(.157)	(.158)	(.171)
.15E+03	(.712E-01)	(.711E-01)	(.714E-01)	(.717E-01)	(.715E-01)	(.713E-01)	(.716E-01)	(.721E-01)	(.779E-01)
.20E+03	(.405E-01)	(.404E-01)	(.406E-01)	(.408E-01)	(.406E-01)	(.405E-01)	(.407E-01)	(.410E-01)	(.443E-01)
.30E+03	(.181E-01)	(.181E-01)	(.182E-01)	(.183E-01)	(.182E-01)	(.182E-01)	(.182E-01)	(.184E-01)	(.198E-01)
.40E+03	(.102E-01)	(.102E-01)	(.103E-01)	(.103E-01)	(.103E-01)	(.102E-01)	(.103E-01)	(.104E-01)	(.112E-01)
.50E+03	(.656E-02)	(.654E-02)	(.657E-02)	(.660E-02)	(.658E-02)	(.657E-02)	(.659E-02)	(.664E-02)	(.716E-02)
.60E+03	(.456E-02)	(.455E-02)	(.457E-02)	(.459E-02)	(.457E-02)	(.456E-02)	(.458E-02)	(.461E-02)	(.498E-02)
.80E+03	(.256E-02)	(.256E-02)	(.257E-02)	(.258E-02)	(.257E-02)	(.257E-02)	(.258E-02)	(.260E-02)	(.280E-02)
.10E+04	(.164E-02)	(.164E-02)	(.165E-02)	(.165E-02)	(.165E-02)	(.164E-02)	(.165E-02)	(.166E-02)	(.179E-02)

[a] LIQUID WATER E<15 KEV : CALCULATED FROM EXPERIMENTAL VALUES OF NARTEN AND LEVY (1971)

[b] LIQUID WATER E>15 KEV : CALCULATED FROM EXPERIMENTAL VALUES OF NARTEN AND LEVY (1971) AND THEORICAL VALUES OF HUBBELL AND OVERBO (1979)

[c] MOLECULAR WATER : CALCULATED FROM THEORICAL VALUES OF BLUM (1971) AND HUBBELL AND OVERBO (1979)

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