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TEMPERATURE-AND DENSITY-DEPENDENT
X-RAY SCATTERING IN A LOW-Z PLASMA

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ABSTRACT

A computer program is described which calculates temperature- and density-dependent differential and total coherent and incoherent x-ray scattering cross sections for a low-Z scattering medium. Temperature and density are arbitrary within the limitations of the validity of local thermodynamic equilibrium, since ionic populations are calculated under this assumption. Scattering cross sections are calculated in the form factor approximation. The scattering medium may consist of any mixture of elements with $Z < 8$, with this limitation imposed by the availability of atomic data.

I. INTRODUCTION

In the calculation of radiative opacities it is usually assumed that scattering is due to free electrons, described by the Thomson and Klein-Nishina cross sections for low-energy and high-energy photons, respectively. The reason that this has been considered satisfactory is that under conditions in which there is an appreciable population of electrons in bound states, absorption processes would be expected to dominate. In this approximation the scattering cross section per atom is simply proportional to the number of electrons, bound or free, per atom.

However, at low photon energies, scattering by bound electrons is coherent, proportional to the square of the number of bound electrons per atom. Thus, in the transition from a plasma consisting of free electrons and totally stripped ions to one consisting of partially ionized atoms, as the number of ions with two or more bound electrons becomes appreciable, the scattering cross section at low energies will begin to increase.

In addition to its possible effect on monochromatic and mean opacities, scattering by bound electrons is of interest in its own right. In transport

calculations, as opposed to diffusion, it would be of some interest to know the degree of departure of the true phase function from the Rayleigh phase (Thomson cross section) describing scattering by free electrons. This requires a knowledge of the differential scattering cross sections for each ion present. The departure of the differential coherent scattering cross section from the Thomson cross section with increasing energy is illustrated in Fig. 1 for neutral lithium.¹ Probably the most direct application of the work described here is in the calculation of the response of x-ray scatterers. If the x-ray flux falling on the scatterer is intense enough, the scatterer may become heated to such an extent that the effect of ionization on the scattering cross sections must be considered. The magnitude of this effect is illustrated in Figs. 2 and 3, which show the coherent, incoherent and total scattering cross sections for neutral and four-times ionized carbon as functions of energy. Also shown is the energy-independent Thomson cross section.

This report describes a computer program which calculates differential (energy- and angle-dependent) and total (energy-dependent) coherent and incoherent scattering cross sections for a low-Z x-ray

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Fig. 1. Differential coherent scattering cross section for neutral lithium as a function of photon energy and scattering angle.

Fig. 2. X-ray scattering cross sections for neutral carbon.

scattering medium at arbitrary temperature and density. The scatterer may consist of any mixture of elements with $Z \leq 8$. This limitation is due to the lack of atomic data for heavier elements. The only input required is the temperature and density, and a description of the mixture in terms of either number fraction or weight fraction. The code then calculates ionic populations under the assumption

Fig. 3. X-ray scattering cross sections for four-times ionized carbon.

of local thermodynamic equilibrium by means of the Saha equation, making use of the Stewart and Pyatt model for pressure ionization.² Coherent and incoherent scattering cross sections are calculated in the form factor approximation. The analytic Hartree-Fock wave functions of Clementi^{3, 4} are used for coherent scattering, while for incoherent scattering values obtained from variational wave functions are used wherever possible.

II. IONIC POPULATIONS

A. Methods Used

Ionic populations are calculated by methods essentially those of Stewart and Pyatt as used in the DIAPHANOUS code,² with certain modifications introduced by Waltz and Wilson in CONFIG, the ILL version of this code.⁵ Both of these are explicit ion codes, the basic difference being that DIAPHANOUS requires an input set of energy levels, while CONFIG calculates hydrogenic statistical weights and energy levels using the screening constants of Mayer.⁶

This latter is the scheme used in the present study. The code actually calculates populations of excited states as well as the ground state for each ion, using the Saha-Boltzmann equation. However, the excited states are lumped together with the ground state in calculating scattering, since the populations of excited states are generally much smaller than that of the ground state. The reason

this was done is to maintain as much commonality as possible with the version of this code which calculates monochromatic and mean opacities as well as temperature dependent scattering cross sections. This code will be described in a separate report.

B. Statistical Weights

Since the electron states are assumed to be strictly hydrogenic, there is no dependence on angular momentum quantum numbers and the statistical weight g for each configuration is given by the product of binomial coefficients

$$g = \prod_n \binom{2n^2}{m_n}, \quad (1)$$

where n is the principal quantum number of each level and m_n is the number of electrons in this level. In the present version of the code n ranges from 1 to 9. The upper limit of 9 was found to be more than adequate during the development of the opacity plus scattering version of the code mentioned above.

C. Energy Levels

In the hydrogenic approximation the total energy, in rydbergs, of the k th configuration is simply

$$E_k = - \sum_{n=1}^9 \frac{m_n \bar{Z}_n^2}{n^2}, \quad (2)$$

where m_n is again the number of electrons in the level with principal quantum number n and $\bar{Z}_n$ is an effective charge seen by an electron in this level. It is given by

$$\bar{Z}_n = Z - \sum_{n'=1}^{n-1} m_{n'} \sigma_{n'n} - \frac{1}{2} (m_n - 1) \sigma_{nn}. \quad (3)$$

where the screening constants $\sigma_{n'n}$ are those tabulated by Mayer.⁶ These screening constants are also used in the XSNB opacity code.^{7,8}

D. Populations

Once the statistical weights g_i and energy levels E_i have been determined the equilibrium population P_i of the i th state is given by the Saha-Boltzmann equation as

$$P_i = g_i \exp \left(\alpha f_i - \frac{E_i}{kT} + \sum_{f=0}^{f_i-1} J_f \right), \quad (4)$$

where J_f is the pressure lowering of the ionization potential of the ionic species with charge f . The net charge of the ion to which state i belongs is f_i and the degeneracy parameter α is given by $\alpha = \ln \Gamma$ where

$$\Gamma = \frac{2(2\pi m kT)^{3/2}}{h^3 N_e} \quad (5)$$

in which kT is expressed in keV, m is the electron mass, h is Planck's constant and N_e is the number density of free electrons. The number of free electrons in turn depends on the populations of the various ionization states as given by Eq. (4). The set of equations represented by Eq. (4) is thus seen to be a set of coupled nonlinear equations. In the work described here these are solved by a straightforward iterative procedure in terms of the parameter Γ . Convergence is quite rapid except at values of kT less than approximately 2 or 3 eV. This is not a serious handicap since at these low temperatures ionization has a very small effect on the scattering cross sections and the values for the neutral species can be used. The pressure lowering J_f is calculated by the methods described by Stewart and Pyatt.²

Figure 4 illustrates the results of a calculation of the populations of the various ionization states of carbon as a function of temperature at a density of 0.036 g/cm³.

III. SCATTERING CROSS SECTIONS

A. The Form Factor Approximation

In the form factor approximation,⁹ which is valid except at very low energies, the cross section for coherent photon scattering by an ion with N bound electrons is given by

Fig. 4. Ionic populations of carbon as a function of temperature for density of 0.036 g/cm³. Number adjacent to each curve denotes number of bound electrons.

$$d\sigma_c = I_c |F(K)|^2 d\Omega, \quad (6)$$

where I_c is the Thomson cross section. The effect of atomic structure on the scattering process is contained in the atomic form factor

$$F(K) = \sum_{j=1}^N \langle \psi_0 | \exp(i\vec{k} \cdot \vec{r}_j) | \psi_0 \rangle \quad (7)$$

in which ψ_0 is the ground state wave function of the scattering ion, $\hbar\vec{k}$ is the momentum transfer, and $\vec{r}_j$ is the radius vector from the nucleus to the j th electron.

In the same approximation, the cross section for incoherent, or Compton, scattering is

$$d\sigma_i = I_c N S(K) d\Omega, \quad (8)$$

where I_c is the Klein-Nishina cross section and

$$S(K) = N^{-1} \left[\sum_{j,k=1}^N \langle \psi_0 | \exp[i\vec{k} \cdot (\vec{r}_j - \vec{r}_k)] | \psi_0 \rangle - |F(K)|^2 \right] \quad (9)$$

is the incoherent scattering function, or Compton scattering factor, the two-electron counterpart of the atomic form factor.

Since the atomic form factor and incoherent scattering function depend on the wave function used to represent the ground state of the target

atom, they can be expected to be sensitive to the degree of refinement of this wave function.

B. Approximate Wave Functions for Many-Electron Atoms

Nonrelativistic wave functions for many electron atoms can be ranked according to the degree to which, as approximations to the eigenfunction of the Schroedinger equation, their corresponding eigenvalues approach the experimental eigenvalue, the total energy of the system. There is, as might be expected, a strong correlation between the accuracy of the wave function and the amount of labor involved in obtaining it.

The simplest approximation is perhaps the statistical or Thomas-Fermi model of the atom. Next in order of complexity is the Hartree or self-consistent field method. In its original form this method does not take into account the antisymmetry of the true wave function. This property is usually referred to as exchange because of the form of the integrals arising in calculating it. The Hartree-Fock method represents antisymmetry exactly through the use of a determinant wave function. Intermediate in complexity between the Hartree and Hartree-Fock methods are the Hartree-Slater approximation and the many variations of this method such as that of Herman and Skillman. In these methods the effect of exchange on the total energy of the system is represented by an additional term in the potential of the Hartree equations.

None of the approximations discussed so far considers the effect of electron correlation, or the Coulomb interaction between individual electrons. One way of doing this is with the variational method, by means of which a solution to the many-electron Schroedinger equation can, in principle, be approximated as closely as desired. Because of the labor involved, variational, or correlated, wave functions are available for only a relatively few atoms and ions.

The above discussion is not intended to be complete, but includes only those methods commonly used in the calculation of x-ray scattering factors. There are many other methods of obtaining approximate wave functions and other properties of many electron atoms. Table I summarizes the properties

TABLE I

FORMS OF ψ_0 COMMONLY USED FOR SCATTERING FACTOR CALCULATIONS

ψ_0	Comments
Thomas-Fermi	Statistical Model
Hartree	Self-consistent Field No Exchange No Correlation
Hartree-Slater (Herman Skillman)	Self-consistent Field Exchange Approximate No Correlation
Dirac-Slater	Relativistic Self-consistent Field Exchange Approximate No Correlation
Hartree-Fock	Self-consistent Field Exchange Exact No Correlation
Variational (Configuration Interaction)	Approaches Exact Solution to Many-electron Wave Equation

of wave functions commonly used in x-ray scattering calculations.

C. Dependence of Scattering Factors on Wave Functions

The question of the sensitivity of x-ray scattering factors, coherent and incoherent, to the degree of refinement of the wave function used, has been investigated for ions with from two through six bound electrons.^{10, 11, 12, 13, 14} It is found that for both coherent and incoherent scattering there does seem to be convergence toward a "best" value as the quality of the wave function is improved.^{12, 13}

Coherent scattering is quite sensitive to exchange, but not to correlation. The use of a Hartree-Fock rather than Hartree-Slater wave function can make a difference of more than 10% in the atomic form factor. However, it has been found that for all practical purposes it is not necessary to use correlated wave functions in the calculation of coherent scattering, since the extra effort required generally results in an additional improvement of less than one percent.

Incoherent scattering, on the other hand, is quite sensitive to the effects of correlation. For

example, for neutral beryllium, there are differences of as much as 30% between values obtained with variational wave functions and the Hartree-Fock values.

Examples of these effects are shown in Figs. 5 and 6 for neutral carbon. The variational wave functions are the configuration-interaction function of Weiss.¹⁵ These consist of expansions of 5, 21, and 40 terms, with the leading term being a variational fit of an analytic function to the Hartree-Fock wave function.

Figures 7 and 8, taken from Ref. 9, show some comparisons with experimental values,^{16, 17} and with other calculations,^{18, 19} In spite of the ready availability of Hartree-Fock wave functions, the Thomas-Fermi model is still widely used for the calculation of atomic form factors. Figure 7 shows that this can lead to errors of as much as 50% for intermediate values of the momentum transfer and factors of two or more at large values of the momentum transfer.

Fig. 5. Comparison of calculated form factors for neutral carbon. $|\Delta F|$ is the absolute value of the difference between the value calculated with the indicated wave function and the value F_{40} calculated with a 40-term configuration-interaction wave function.

Fig. 6. Comparison of calculated incoherent scattering functions for neutral carbon. $|\Delta S|$ is the absolute value of the difference in $S(K)$ analogous to $|\Delta F|$ in Fig. 5.

D. Calculation of Scattering Factors

For the coherent scattering part of the present study, analytic Hartree-Fock wave functions were used since they are available for all neutral atoms and a large number of ions with $Z = 2 - 54$ (Ref. 3, 4). They are also quite straightforward to use, since the integrals required for the calculation of the expectation value in Eq. (7) can be evaluated

Fig. 7. Comparison of calculated and measured atomic form factor for Be (from Ref. 9). Experimental values are from Ref. 16, curve labeled Present is from Ref. 11, and curve labeled T.F. represents Thomas-Fermi values from Ref. 18.

Fig. 8. Comparison of calculated and measured atomic form factor for Be (from Ref. 9). Experimental values are from Ref. 17, curve labeled Present is from Ref. 13, and curve labeled Cromer is from Ref. 19.

in closed form.¹⁰ The methods used for calculating coherent scattering cross sections are described in Appendix A.

Incoherent scattering cross sections used in this study were calculated with incoherent scattering functions obtained with variational wave functions, when available. In other cases Hartree-Fock values were used.^{20, 21} For two ions, singly and doubly ionized nitrogen, isoelectronic interpolation had to be resorted to. Sources of the incoherent scattering functions used are given in Table II. Values are listed in Appendix 2. Except for neutral atoms and hydrogenic ions, and two-electron ions for $Z = 7$ and 10, Table II summarizes the present status of available atomic data. This is the reason for the limitation to ions with $Z \leq 8$.

TABLE II

SOURCES OF INCOHERENT SCATTERING FUNCTIONS

Z	n/e							
	1	2	3	4	5	6	7	8
1	A							
2	A	V						
3	A	V	V					
4	A	V	V	V				
5	A	V	V	V	V			
6	A	V	V	V	V	V		
7	A	V	V	V	I	I	H	
8	A	V	V	V	H	H	H	H

A - Analytic expression (Eqs. 10 and 11)
V - Variational wave functions (Refs. 10 - 14)
H - Hartree-Fock (Refs. 20 and 21)
I - Interpolation

For both coherent and incoherent scattering by one-electron ions analytic expressions are readily obtained when hydrogenic ground-state wave functions are substituted in Eqs. (7) and (9). These are:

$$F(K) = [1 + (Ka_0/2Z)^2]^{-2} \quad (10)$$

and

$$S(K) = 1 - [F(K)]^2 \quad (11)$$

for the form factor and incoherent scattering function, respectively. In Eqs. (10) and (11) the momentum transfer is expressed in terms of the dimensionless combination Ka_0 where a_0 is the Bohr radius. Use of this variable is convenient in computational work, but for purposes of comparing with experiment it is necessary to express the momentum in terms of the scattering angle θ and either the photon energy or wavelength. In terms of the scattering angle and wavelength the magnitude of the momentum transfer is

$$K = 4\pi(\sin \frac{1}{2} \theta)/\lambda. \quad (12)$$

Values of the incoherent scattering function tabulated in Appendix B are given as functions of the variable $(\sin \frac{1}{2} \theta)/\lambda$, rather than Eq. (12), since this is the variable generally used in tabulating x-ray scattering factors.

IV. RESULTS

The computer program SCION (Scattering by Ions) described here has been extensively tested for two commonly used scattering materials, carbon and lithium hydride. It has also been used to investigate the scattering contribution to the opacity of several mixtures of astrophysical interest,²² and to study the effect of ionization on x-ray scattering in air. In this latter case the effect of argon had to be neglected. This is not a bad approximation since scattering, unlike absorption, is relatively insensitive to the presence of small amounts of high-Z elements.

In Fig. 9 is shown the differential coherent scattering cross section for carbon as a function of energy and angle at density of 0.18 g/cm^3 and $kT = 40 \text{ eV}$. Figure 10 shows the differential incoherent scattering cross section for lithium hydride at a density of 0.82 g/cm^3 and $kT = 40 \text{ eV}$.

Fig. 9. Differential coherent scattering cross section for carbon at density 0.18 g/cm^3 and $kT = 40 \text{ eV}$.

Integration of the differential cross sections over angle is carried out by means of 64-point Gaussian quadrature.²³ The result is a set of total cross sections as a function of photon energy. Figure 11 shows these cross sections for carbon at density 0.018 g/cm^3 and $kT = 5 \text{ eV}$. This amount of heating has reduced the low-energy limit of the scattering cross section by approximately 25%.

Fig. 10. Differential incoherent scattering cross section for lithium hydride at density 0.82 g/cm^3 and $kT = 40 \text{ eV}$.

Fig. 11. Total scattering cross sections for carbon at density 0.018 g/cm³ and $kT = 50$ V.

This change in the low-energy limit of the total scattering cross section is a useful measure of the effect of heating on the scattering cross section. In a totally stripped plasma this is just the Thomson cross section, which in cm²/g is approximately $0.4 \langle Z \rangle / \langle A \rangle$ where $\langle Z \rangle$ and $\langle A \rangle$ are the average atomic number and atomic weight of the mixture, respectively. For a mixture containing only neutral atoms this limit becomes $0.4 \langle Z^2 \rangle / \langle A \rangle$ cm²/g. Figure 12 shows the results of an extensive study of the behavior as a function of temperature and density of the low energy scattering limit for carbon. This is expressed as the ratio of the actual cross section to the Thomson cross section. For carbon this ratio should

Fig. 12. Ratio of the low-energy limit of the true carbon scattering cross section to the Thomson cross section.

approach 6.0 at low temperature. At high temperatures the ratio approaches 1.0. From Fig. 12 it can be seen that for kT greater than approximately 100 to 150 eV, the Thomson cross section gives an adequate description of the scattering process. Figure 13 shows the results of a similar study for air.

Fig. 13. Ratio of the low-energy limit of the true scattering cross section for air to the Thomson cross section.

APPENDIX A: CALCULATION OF ATOMIC FORM FACTORS

The Clementi analytic Hartree-Fock wave function ψ for an n -electron atom is represented by the $n \times n$ Slater determinant

$$\psi = |\phi_{1s}^2 \phi_{2s}^2 \phi_{2p}^6 \dots| \quad (A-1)$$

in which the one-electron functions are the linear combinations

$$\phi_{nl} = \sum_i c_i(n,l) \psi_{nl}^i(r, \theta, \phi). \quad (A-2)$$

The coefficients $c_i(n,l)$ are determined by a Gram-Schmidt orthogonalization procedure and the function ψ_{nl} are the Slater-type orbitals

$$\psi_{nlm} = \frac{1}{[(2n)!]^{1/2}} (2\xi)^{n+1/2} r^{n-1} e^{-\xi r} Y_{lm}(\theta, \phi). \quad (A-3)$$

The parameters ξ are nonlinear variational parameters with respect to which the total energy is minimized, providing an analytic approximation to the Hartree-Fock function. Although the magnetic quantum number m appears in the definition of the Slater orbitals, for the purpose of calculating atomic form factors it is not necessary to carry this dependence explicitly in the definition of the functions.

The plane wave in Eq. (2) may be written as the spherical harmonic expansion

$$\exp(i\vec{k} \cdot \vec{r}) = \sum_L i^L [4\pi(2L+1)]^{1/2} j_L(Kr) Y_{L0}(\hat{r}) \quad (A-4)$$

where $j_L(Kr)$ is a spherical Bessel function.²⁴ Because of the orthonormality of the single-particle functions given by Eq. (A-2), the atomic form factor for an atom containing electrons in n subshells is

$$F(K) = \sum_{i=1}^n N_i \langle n_i l_i m_i | \exp(i\vec{k} \cdot \vec{r}) | n_i l_i m_i \rangle, \quad (A-5)$$

where N_i are the occupation numbers for the various subshells appearing in the exponents in Eq. (A-1). When Eq. (A-4) is substituted in Eq. (A-5) and the integration over angles carried out, it is found that each integral in the sum is given by

$$\langle n l | \exp(i\vec{k} \cdot \vec{r}) | n l \rangle = \sum_{\ell} \underline{C}(n, \ell) \underline{M}(n, \ell) \underline{C}(n, \ell), \quad (A-6)$$

where $\underline{C}(n, \ell)$ is the vector of coefficients in the expression Eq. (A-2) and the matrix $\underline{M}(n, \ell)$ has elements

$$M_{ij} = \int_0^\infty R_{n_i}(\xi_i r) j_0(Kr) R_{n_j}(\xi_j r) r^2 dr, \quad (A-7)$$

where R_n is the radial part of the Slater orbital given by Eq. (A-3). When these radial functions are substituted in Eq. (A-7), the integral is seen to be a special case of the more general one described previously for spherical Bessel functions, powers of r , and exponentials.¹⁰ It is

$$M_{ij} = \frac{I_{ij}}{2(n_i+n_j)(1+a^2)} \left[\frac{1+(1+a^2)^{1/2}}{2(1+a^2)} \right]^{n_i+n_j-1} \quad (A-8)$$

$$\times \sum_{k=0}^{n_i+n_j-1} \binom{2n_i+2n_j}{2k+1} \left[\frac{1-(1+a^2)^{1/2}}{1+(1+a^2)^{1/2}} \right]^{1/2}$$

in which $a = K/(\xi_i + \xi_j)$ and I_{ij} is the integral

$$I_{ij} = \int_0^\infty R_{n_i}(\xi_i r) R_{n_j}(\xi_j r) r^2 dr \quad (A-9)$$

which has also been described previously.²⁵ When the radial functions given by Eq. (A-3) are substituted in Eq. (A-9) the result is

$$\frac{(2\xi_i)^{n_i+1/2} (2\xi_j)^{n_j+1/2}}{[(2n_i)! (2n_j)!]^{1/2}} \int_0^\infty r^{n_i+n_j} e^{-(\xi_i+\xi_j)r} dr \quad (A-10)$$

$$= \left(\frac{2}{\xi_i + \xi_j} \right)^{n_i+n_j+1} \xi_i^{n_i} \xi_j^{n_j} (n_i+n_j)! \left[\frac{\xi_i \xi_j}{(2n_i)! (2n_j)!} \right]^{1/2}.$$

APPENDIX B. INCOHERENT SCATTERING FUNCTIONS

$\sin(\theta/2)/\lambda$ ($\text{\AA}^{-1}$)	He I	Li II	Be III	B IV	C V	N VI	O VII	Li I	Be II	B III	C IV	N V	O VI
0.05	0.08	0.04	0.02	0.01	0.005	0.003	0.002	0.50	0.22	0.12	0.075	0.05	0.04
0.10	0.30	0.13	0.07	0.04	0.03	0.02	0.01	1.03	0.65	0.41	0.27	0.19	0.14
0.15	0.58	0.26	0.12	0.09	0.06	0.04	0.03	1.25	1.00	0.73	0.53	0.39	0.30
0.20	0.88	0.42	0.23	0.16	0.10	0.07	0.05	1.42	1.20	0.99	0.78	0.61	0.48
0.25	1.15	0.62	0.36	0.24	0.15	0.12	0.09	1.60	1.35	1.17	0.98	0.81	0.66
0.30	1.36	0.81	0.50	0.33	0.22	0.18	0.12	1.80	1.48	1.30	1.14	0.98	0.84
0.35	1.53	1.00	0.64	0.43	0.30	0.23	0.17	1.98	1.61	1.41	1.26	1.12	0.98
0.40	1.66	1.15	0.77	0.53	0.39	0.30	0.22	2.14	1.75	1.51	1.36	1.23	1.11
0.45	1.75	1.30	0.91	0.64	0.48	0.36	0.28	2.29	1.89	1.62	1.45	1.32	1.21
0.50	1.82	1.43	1.04	0.75	0.57	0.42	0.33	2.42	2.02	1.73	1.54	1.40	1.29
0.60	1.90	1.63	1.27	0.96	0.74	0.58	0.46	2.61	2.25	1.94	1.72	1.55	1.44
0.70	1.95	1.75	1.46	1.16	0.91	0.74	0.60	2.75	2.44	2.13	1.89	1.70	1.57
0.80	1.97	1.84	1.61	1.33	1.09	0.88	0.72	2.83	2.59	2.30	2.05	1.85	1.70
0.90	1.98	1.89	1.71	1.47	1.25	1.03	0.86	2.89	2.70	2.45	2.21	1.99	1.83
1.00	1.99	1.92	1.79	1.58	1.37	1.16	0.99	2.93	2.78	2.57	2.34	2.13	1.95
1.10	2.00	1.95	1.85	1.67	1.49	1.28	1.10	2.95	2.84	2.66	2.46	2.25	2.07
1.20	2.00	1.97	1.89	1.76	1.58	1.40	1.21	2.97	2.88	2.74	2.56	2.36	2.18
1.30	2.00	1.98	1.92	1.81	1.66	1.50	1.32	2.98	2.92	2.80	2.64	2.46	2.29
1.40	2.00	1.98	1.94	1.85	1.72	1.58	1.42	2.98	2.94	2.84	2.71	2.55	2.38
1.50	2.00	1.99	1.96	1.89	1.78	1.65	1.49	2.99	2.95	2.88	2.76	2.62	2.46
1.60	2.00	2.00	1.97	1.92	1.82	1.71	1.56	2.99	2.96	2.91	2.81	2.68	2.54
1.80	2.00	2.00	1.98	1.95	1.88	1.80	1.68	3.00	2.98	2.94	2.88	2.78	2.66
2.00	2.00	2.00	2.00	1.97	1.93	1.86	1.77	3.00	2.99	2.96	2.92	2.85	2.75
2.20	2.00	2.00	2.00	1.98	1.95	1.89	1.84	3.00	3.00	2.98	2.95	2.89	2.82
2.40	2.00	2.00	2.00	1.99	1.96	1.93	1.88	3.00	3.00	2.99	2.96	2.93	2.87
2.60	2.00	2.00	2.00	2.00	1.98	1.96	1.92	3.00	3.00	2.99	2.98	2.95	2.91
2.80	2.00	2.00	2.00	2.00	1.99	1.97	1.94	3.00	3.00	3.00	2.98	2.96	2.93
3.00	2.00	2.00	2.00	2.00	2.00	1.98	1.95	3.00	3.00	3.00	2.99	2.97	2.95
3.50	2.00	2.00	2.00	2.00	2.00	2.00	2.00	3.00	3.00	3.00	3.00	3.00	3.00

$\sin(\theta/2)/\lambda$ ($\text{\AA}^{-1}$)	Be I	B II	C III	N IV	O V	B I	C II	N III	O IV	C I	N II	O III	N I	O II	O I
0.05	0.40	0.20	0.13	0.08	0.06	0.36	0.19	0.15	0.10	0.31	0.25	0.20	0.30	0.45	0.45
0.10	1.17	0.70	0.46	0.32	0.23	1.15	0.69	0.50	0.36	1.04	0.70	0.46	0.63	1.05	0.97
0.15	1.77	1.25	0.88	0.65	0.49	1.93	1.31	1.05	0.77	1.87	1.40	1.00	1.35	1.90	1.90
0.20	2.12	1.70	1.31	1.01	0.78	2.53	1.91	1.55	1.24	2.60	2.05	1.59	2.05	2.82	2.80
0.25	2.32	2.01	1.66	1.35	1.10	2.93	2.39	2.03	1.75	3.20	2.65	2.25	2.85	3.55	3.80
0.30	2.47	2.22	1.93	1.64	1.38	3.19	2.76	2.40	2.18	3.64	3.17	2.79	3.43	4.08	4.30
0.35	2.61	2.37	2.13	1.88	1.63	3.36	3.03	2.78	2.51	3.96	3.60	3.30	3.95	4.59	4.80
0.40	2.74	2.49	2.28	2.06	1.84	3.45	3.23	3.00	2.83	4.18	3.90	3.61	4.36	4.78	5.27
0.45	2.88	2.61	2.41	2.21	2.01	3.62	3.38	3.20	3.05	4.35	4.12	3.90	4.65	5.02	5.60
0.50	3.00	2.71	2.51	2.33	2.15	3.73	3.50	3.32	3.19	4.48	4.27	4.06	4.90	5.18	5.84
0.60	3.24	2.92	2.69	2.52	2.36	3.95	3.70	3.52	3.39	4.69	4.50	4.32	5.22	5.44	6.18
0.70	3.43	3.11	2.87	2.68	2.53	4.15	3.88	3.70	3.54	4.88	4.68	4.50	5.44	5.64	6.42
0.80	3.58	3.29	3.03	2.82	2.66	4.32	4.05	3.85	3.70	5.05	4.80	4.65	5.61	5.82	6.61
0.90	3.69	3.43	3.18	2.97	2.80	4.47	4.21	4.00	3.81	5.21	4.95	4.79	5.77	5.97	6.76
1.00	3.78	3.56	3.32	3.10	2.92	4.59	4.34	4.12	3.95	5.35	5.10	4.93	5.91	6.12	6.90
1.10	3.84	3.65	3.44	3.22	3.04	4.69	4.46	4.25	4.06	5.47	5.25	5.05	6.04	6.25	7.04
1.20	3.88	3.73	3.54	3.34	3.15	4.76	4.57	4.35	4.18	5.57	5.35	5.17	6.15	6.37	7.12
1.30	3.91	3.79	3.62	3.44	3.26	4.82	4.65	4.45	4.30	5.66	5.45	5.26	6.25	6.50	7.22
1.40	3.94	3.84	3.70	3.52	3.35	4.86	4.72	4.55	4.42	5.72	5.55	5.37	6.35	6.57	7.31
1.50	3.95	3.88	3.75	3.60	3.44	4.90	4.78	4.63	4.50	5.78	5.62	5.45	6.47	6.65	7.37
1.60	3.97	3.90	3.80	3.67	3.51	4.92	4.82	4.70	4.57	5.83	5.68	5.52	6.50	6.75	7.45
1.80	3.98	3.94	3.87	3.77	3.64	4.95	4.89	4.75	4.68	5.89	5.78	5.62	6.65	6.85	7.60
2.00	3.99	3.96	3.92	3.84	3.74	4.97	4.93	4.82	4.75	5.93	5.82	5.70	6.80	6.95	7.67
2.20	3.99	3.98	3.94	3.89	3.81	4.98	4.96	4.90	4.85	5.95	5.85	5.74	6.87	7.00	7.77
2.40	4.00	3.99	3.96	3.92	3.86	4.99	4.97	4.93	4.90	5.97	5.87	5.77	6.92	7.00	7.85
2.60	4.00	3.99	3.97	3.95	3.90	5.00	4.98	4.95	4.93	5.98	5.89	5.80	6.97	7.00	7.90
2.80	4.00	4.00	3.98	3.96	3.93	5.00	4.99	4.97	4.95	5.99	5.91	5.85	6.99	7.00	7.95
3.00	4.00	4.00	3.99	3.97	3.95	5.00	5.00	4.99	4.97	6.00	5.93	5.90	7.00	7.00	8.00
3.50	4.00	4.00	4.00	4.00	4.00	5.00	5.00	5.00	5.00	6.00	6.00	6.00	7.00	7.00	8.00

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