

Anomalous Dispersion Corrections Computed from Self-Consistent Field Relativistic Dirac-Slater Wave Functions*

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(Received 23 December 1963 and in revised form 8 October 1964)

Anomalous dispersion terms, $\Delta f'$ and $\Delta f''$, have been computed for elements number 10 through 98 for five commonly used X-ray wavelengths. Oscillator strengths were calculated from self-consistent field relativistic Dirac wave functions which included in the potential Slater's approximate exchange contribution and Latter's self-interaction term.

Introduction

In recent years, as counter devices have come into common use, it has been routinely possible to measure the effects of anomalous dispersion in X-ray diffraction experiments. The importance of this effect has been pointed out by Templeton (1955). Dauben & Templeton (1955) have published values of the anomalous dispersion corrections for most of the elements, as calculated by the method of Parratt & Hempstead (1954). An extension of Dauben & Templeton's (1955) calculations is given in *International Tables for X-Ray Crystallography* (1962). These calculations require a knowledge of the oscillator strengths and the manner in which the photoelectric absorption coefficient varies with the wavelength of the incident X-ray. An attempt has been made to improve the previous calculations by using atomic wave functions to obtain the oscillator strengths.

Initially, the Hartree wave functions recently computed by Boyd, Larson & Waber (1963) were used for calculation of the oscillator strengths. It was soon clear that, for heavy elements in particular, wave functions obtained by the simple Hartree model were completely inadequate for this purpose. The method was then checked with wolfram and uranium relativistic wave functions which had been calculated by Cohen (1960), and the results were considerably improved. Then, relativistic wave functions, which had been computed by Liberman, Waber & Cromer (1965), became available for all atoms. These relativistic wave functions include Slater's (1951, 1960) approximate exchange correction, and Latter's (1955) self-interaction term; hence we call them Dirac-Slater (DS) wave functions. The final set of oscillator strengths and dispersion terms in this paper was obtained from these DS wave functions.

* Work performed under the auspices of the U.S. Atomic Energy Commission.

Theory

The theoretical treatment as given by James (1948) will be summarized. The total atomic scattering factor, f , is in general complex and is given by

$$f = f_0 + \Delta f' + i\Delta f'' \quad (1)$$

where f_0 is the atomic scattering factor for radiation with frequency much higher than any absorption edge and $\Delta f'$ and $\Delta f''$ are the real and imaginary components of the anomalous dispersion. Neglecting damping, which is of importance only when the incident frequency is within about 10^{-4} of an absorption edge (Parratt & Hempstead, 1954), $\Delta f'$ is given by

$$\Delta f' = \sum_k \int_{\omega_k}^{\infty} \frac{\omega^2 (dg/d\omega)_k}{\omega_i^2 - \omega^2} d\omega \quad (2)$$

where the summation is over all the absorption edges and

ω_k = frequency of the absorption edge,

ω_i = incident frequency,

$(dg/d\omega)_k$ = oscillator density of type k at frequency ω ,

$(dg/d\omega)_k d\omega$ = the number of virtual oscillators of type k having frequencies between ω and $\omega + d\omega$.

The imaginary component, $\Delta f''$, is given by

$$\Delta f'' = \frac{1}{2}\pi\omega_i \sum_k (dg/d\omega)_{k_i} \quad (3)$$

where the summation is again over all of the absorption edges.

If we knew the functions $(dg/d\omega)_k$ we could calculate $\Delta f'$ and $\Delta f''$ directly from equations (2) and (3). These functions are not known, although Hönl (1933) has made satisfactory calculations for the K electrons assuming them to be hydrogen-like. Hönl has also

Table 1. Calculation of oscillator strengths for uranium

Transition	$g_{n'l'}^{n'l} \times 10^4$			Coordinate matrix element $\langle r \rangle$			Wavelength of transition				
	H	HD	DS	H	HD	DS	H	HD	DS	Observed	
$1s\frac{1}{2} \rightarrow 2p\frac{1}{2}$	1409	972	977	1.358-2*	1.116-2	1.121-2	0.1325 Å	0.1297 Å	0.1302 Å	0.1310 Å	
	2898	1924	1937	1.358-2	1.089-2	1.094-2	0.1288	0.1247	0.1251	0.1260	
	225	127	126	5.027-3	3.736-3	3.727-3	0.1139	0.1113	0.1116	0.1123	
	452	338	340	5.027-3	4.294-3	4.314-3	0.1133	0.1104	0.1107	0.1114	
	53	29	29	2.398-3	1.761-3	1.759-3	0.1100	0.1075	0.1078	0.1084	
	106	81	83	2.398-3	2.075-3	2.101-3	0.1099	0.1073	0.1076	0.1082	
	12	7	7	1.153-3	8.408-4	8.469-4	0.1091	0.1066	0.1069	} 0.1074	
	25	19	19	1.153-3	9.925-4	1.012-3	0.1091	0.1066	0.1068		
	2	1	1	4.432-4	3.361-4	3.541-4	0.1089	0.1065	0.1066		
	$6p\frac{1}{2}$	3	3	3	4.432-4	3.767-4	4.069-4	0.1089	0.1064	0.1066	
$2s\frac{1}{2} \rightarrow 2p\frac{1}{2}$	156	135	142	-6.050-2	-4.832-2	-4.806-2	23.7784	17.5177	16.4805		
	1924	2252	2263	-6.050-2	-5.505-2	-5.477-2	3.8523	2.7245	2.6842		
	1260	1055	1082	3.120-2	2.795-2	2.823-2	0.7824	0.7494	0.7462	0.7479	
	2611	866	899	3.120-2	1.744-2	1.773-2	0.7552	0.7118	0.7081	0.7102	
	227	187	190	1.188-2	1.060-2	1.063-2	0.6300	0.6074	0.6038	0.6042	
	456	190	198	1.188-2	7.510-3	7.642-3	0.6270	0.6007	0.5970	0.5988	
	50	41	42	5.446-3	4.830-3	4.866-3	0.6018	0.5798	0.5756	0.5766	
	100	43	45	5.446-3	3.497-3	3.573-3	0.6017	0.5783	0.5741	0.5750	
	7	6	7	2.076-3	1.912-3	2.012-3	0.5968	0.5740	0.5696	} 0.5706	
	15	6	7	2.076-3	1.321-3	1.428-3	0.5968	0.5738	0.5694		
$2p\frac{1}{2} \rightarrow 1s\frac{1}{2}$	-1409	-972	-977	1.358-2	1.116-2	1.121-2	0.1325	0.1297	0.1302		
	-156	-135	-137	-6.050-2	-4.832-2	-4.723-2	23.7784	17.5177	16.4801		
	161	136	142	1.145-2	1.036-2	1.060-2	0.8238	0.8006	0.7990	0.8052	
	6945	3865	3893	5.074-2	3.704-2	3.710-2	0.7508	0.7188	0.7162	0.7200	
	27	23	24	4.175-3	3.825-3	3.888-3	0.6515	0.6343	0.6318	0.6355	
	946	636	641	1.722-2	1.389-2	1.392-2	0.6351	0.6143	0.6117	0.6148	
	6	5	6	1.953-3	1.784-3	1.816-3	0.6189	0.6014	0.5982	0.6011	
	165	112	116	7.079-3	5.741-3	5.830-3	0.6146	0.5955	0.5922	0.5947	
	1	1	1	8.220-4	7.714-4	8.078-4	0.6125	0.5940	0.5906		
	2	1	2	1.488-3	1.048-3	1.581-3	0.6116	0.5927	0.5892	0.5920	
$7s\frac{1}{2}$	0	0	0	2.230-4	2.209-4	2.622-4	0.6116	0.5927	0.5892		
$2p\frac{3}{2} \rightarrow 1s\frac{1}{2}$	-1449	-962	-969	1.358-2	1.089-2	1.094-2	0.1288	0.1247	0.1251		
	-962	-1126	-1132	-6.050-2	-5.505-2	-5.477-2	3.8523	2.7245	2.6842		
	132	418	430	1.145-2	2.096-2	2.125-2	1.0036	1.0648	1.0641	1.0671	
	581	515	518	5.074-2	4.851-2	4.856-2	0.8973	0.9249	0.9222	0.9224	
	5272	4704	4737	5.074-2	4.855-2	4.863-2	0.8901	0.9128	0.9099	0.9106	
	23	59	59	4.175-3	6.769-3	6.784-3	0.7591	0.7895	0.7868	0.7704	
	82	70	69	1.722-2	1.615-2	1.606-2	0.7369	0.7588	0.7559	0.7566	
	734	681	682	1.722-2	1.682-2	1.680-2	0.7363	0.7569	0.7539	0.7546	
	5	13	13	1.953-3	3.077-3	3.084-3	0.7152	0.7392	0.7354	0.7361	
	14	12	12	7.079-3	6.533-3	6.568-3	0.7095	0.7303	0.7264	} 0.7263	
	129	116	120	7.079-3	6.824-3	6.903-3	0.7094	0.7300	0.7260		
	1	2	3	8.220-4	1.323-3	1.364-3	0.7067	0.7280	0.7239		0.7252
	$6d\frac{3}{2}$	0	0	0	1.488-3	1.189-3	1.774-3	0.7054	0.7261	0.7219	0.7224
	$7s\frac{1}{2}$	0	0	0	2.230-4	3.787-4	4.421-4	0.7054	0.7261	0.7219	

* The notation 1.358-2 means 1.358×10^{-2} .

applied his method to the L electrons but the approximation of hydrogen-like L electrons is not as good. Eisenlohr & Müller (1954) have also applied Hönl's method to the L electrons for several atoms.

It is possible to relate the functions $(dg/d\omega)_k$ to the photoelectric absorption coefficients and to the oscillator strengths and, with certain assumptions regarding the absorption coefficients, perform the integration of equation (2). The total oscillator strength, g_K , for the K continuum is given by

$$g_K = \int_{\omega_K}^{\infty} (dg/d\omega)_K d\omega. \quad (4)$$

The atomic photoelectric absorption coefficient $\mu(\omega)$ is related to $dg/d\omega$ by

$$(dg/d\omega) = (mc/2\pi^2e^2)\mu(\omega) \quad (5)$$

where the symbols m , c and e have their usual meaning. Thus the oscillator density can be determined empirically from experimental values of $\mu(\omega)$.

The variation of $\mu(\omega)$ for a particular edge is fairly well represented by the empirical formula

$$\mu(\omega) = \begin{cases} (\omega_k/\omega)^n \mu(\omega_k) & \text{for } \omega > \omega_k \\ 0 & \text{for } \omega < \omega_k \end{cases} \quad (6)$$

where ω_k is the frequency of the edge, $\mu(\omega_k)$ is the absorption coefficient at the edge, and n has a value of the order of 3. Unfortunately, n varies, depending on the particular edge involved, and is a function of atomic number. Uncertainty in the value of n is a serious defect in the present analysis; further, the assumption made in equation (6) is not strictly valid.

If equations (5) and (6) are substituted into (4) we get

$$\begin{aligned} g_k &= \int_{\omega_k}^{\infty} (mc/2\pi^2e^2)\mu(\omega) d\omega \\ g_k &= \frac{mc}{2\pi^2e^2} \mu(\omega_k) \int_{\omega_k}^{\infty} \left(\frac{\omega_k}{\omega}\right)^n d\omega \\ g_k &= \frac{mc}{2\pi^2e^2} \cdot \frac{\omega_k}{n-1} \mu(\omega_k). \end{aligned} \quad (7)$$

If n and $\mu(\omega_k)$ are determined from experiment, g_k can be calculated from (7). Another method of calculating g_k will be discussed below.

Equations (5) and (6) can be substituted into (2) resulting in

$$\Delta f'_k = \frac{mc}{2\pi^2e^2} \mu(\omega_k) \omega_k^n \int_{\omega_k}^{\infty} \frac{\omega^2 d\omega}{(\omega_i^2 - \omega^2) \omega^n}. \quad (8)$$

Equation (8) has been integrated for the general case by Parratt & Hempstead (1954). These authors give expressions for $\Delta f'_k$ for various values of n as functions of g_k and x , where $x = \omega_i/\omega_k$.

Substitution of equations (5), (6) and (7) in (3) gives

$$\begin{aligned} \Delta f''_k &= \frac{mc}{4\pi e^2} \omega_i \left(\frac{\omega_k}{\omega_i}\right)^n \mu(\omega_k) \\ \Delta f''_k &= \frac{1}{2} \pi \frac{n-1}{x^{n-1}} g_k \end{aligned} \quad (9)$$

where $x = \omega_i/\omega_k$ as before. The dispersion terms for the whole atom are then obtained by using appropriate values of n and summing equations (8) and (9) over all the absorption edges.

Experimental values of $\mu(\omega)$ are not available for all atoms and it is difficult to determine $\mu(\omega)$ with accuracy. Thus there are few experimental values for oscillator strengths. It was therefore decided to calculate these quantities from the Hartree wave functions which have recently been computed.

Table 2. Oscillator strengths for wolfram and uranium

Edge	Wolfram				Uranium			
	H	HD	DS	Hönl	H	HD	DS	Hönl
$1s\frac{1}{2}$	1.04	1.24	1.24	1.15	0.96	1.30	1.30	1.12
$2s\frac{1}{2}$	0.88	1.13	1.10	1.35	0.64	1.04	1.03	1.28
$2p\frac{1}{2}$	0.89	1.25	1.24	3.55	0.66	1.27	1.26	3.22
$2p\frac{3}{2}$	2.31	2.33	2.31		2.18	2.20	2.18	
$3s\frac{1}{2}$	0.83	1.01	1.01		0.51	0.87	0.87	
$3p\frac{1}{2}$	1.15	1.36	1.33	0.78	1.22	1.19		
$3p\frac{3}{2}$	3.15	3.05	2.98	2.93	2.82	2.74		
$3d\frac{3}{2}$	4.67	4.37	4.25	3.97	3.59	3.50		
$3d\frac{5}{2}$	6.57	6.54	6.35	5.42	5.35	5.25		
$4s\frac{1}{2}$	0.86	0.78	0.81	0.60	0.67	0.68		
$4p\frac{1}{2}$	0.89	0.88	0.91	0.69	0.80	0.82		
$4p\frac{3}{2}$	2.43	2.39	2.44	2.61	2.49	2.49		
$4d\frac{3}{2}$	3.17	2.80	2.88	4.18	3.42	2.43		
$4d\frac{5}{2}$	4.45	4.20	4.34	5.78	5.29	5.37		
$4f\frac{5}{2}$	10.76	10.62	10.60	10.74	10.46	10.46		
$4f\frac{7}{2}$	14.56	14.47	14.48	14.13	13.98	13.98		

Table 5. Calculated eigenvalues used as absorption edges in the calculation of $\Delta f'$ and $\Delta f''$

Units are Rydbergs

Atom	Edge														
	$1s\frac{1}{2}$	$2s\frac{1}{2}$	$2p\frac{1}{2}$	$2p\frac{3}{2}$	$3s\frac{1}{2}$	$3p\frac{1}{2}$	$3p\frac{3}{2}$	$3d\frac{5}{2}$	$4s\frac{1}{2}$	$4p\frac{1}{2}$	$4p\frac{3}{2}$	$4d\frac{3}{2}$	$4d\frac{5}{2}$	$4f\frac{5}{2}$	$4f\frac{7}{2}$
Ne	63.077	3.1779	1.4758	1.4672											
Na	78.203	4.7397	2.6769	2.6622											
Mg		6.5757													
Al		8.7498													
Si		11.137													
P		13.754													
S		16.607													
Cl		19.701													
Ar	233.55	23.038	18.334	18.160	2.1259	1.0749	1.0603								
K		27.282													
Ca		31.909													
Sc		36.331													
Ti		40.972													
V		45.846													
Ga		94.871													
Ge		103.06													
As		111.66													
Se		120.65													
Br		130.04													
Kr		139.83													
Tc	1544.7	222.45	205.95	197.08	39.503	33.021	31.518	19.911	19.617						
Xe	2540.1	398.19	375.16	350.93	82.488	72.745	68.098	50.778	49.785						
Pm	3324.1	543.53	515.91	474.17	119.46	107.42	98.966	77.849	75.998	24.114	19.475	17.616	9.5771		
Hg														8.3300	8.0033
Po	6872.2	1244.4	1197.9	1015.5	303.60	282.29	241.14	206.00	197.27	71.465	62.054	51.775	36.384	34.450	14.311
At	7067.1	1285.3	1237.8	1044.7	315.26	293.45	249.75	213.96	204.72	75.148	65.483	54.495	38.721	36.655	15.978
Rn	7266.0	1327.3	1278.7	1074.4	327.23	304.93	258.55	222.07	212.31	78.948	69.023	57.250	41.124	38.920	17.705
Fr	7469.1	1370.6	1321.0	1105.0	339.86	317.06	267.85	230.69	220.39	83.194	73.006	60.475	43.923	41.573	19.819
Ac	7887.8	1460.4	1408.6	1167.3	366.04	342.20	286.90	248.36	239.90	91.966	81.238	66.976	49.636	46.973	24.137
Pa	8322.8	1553.8	1499.7	1230.5	392.65	367.75	305.69	265.76	253.04	100.28	88.998	72.807	54.666	51.658	27.731
Np	8775.6	1651.8	1595.3	1295.4	420.45	394.44	324.90	283.56	269.48	108.86	96.994	78.648	59.696	56.312	31.285
Pu	9008.6	1702.3	1644.5	1328.0	434.48	407.89	334.32	292.27	277.47	112.90	100.74	81.228	61.865	58.279	32.697
Am	9247.0	1754.4	1695.3	1361.5	449.27	422.10	344.28	301.52	285.97	117.45	104.99	84.246	64.470	60.673	34.536
Cm	9490.7	1808.2	1747.8	1395.8	464.85	437.09	354.81	311.32	294.99	122.53	109.76	87.711	67.519	63.503	36.812
Bk	9739.2	1863.0	1801.3	1430.2	480.42	452.05	365.07	320.85	303.72	127.32	114.23	90.815	70.205	65.960	38.710
Cf	9993.1	1919.3	1856.2	1465.0	496.39	467.40	375.48	330.53	312.55	132.23	118.83	93.958	72.926	68.443	40.631

The quantities $g(k, n)$ are the quantum mechanical analogues of the classical oscillator strengths. These quantities are proportional to the transition probability of an electron going from state k to state n and thus are proportional to the coordinate matrix elements. The Thomas-Reiche-Kuhn sum rule states that for a one-electron atom,

$$\sum_n g(k, n) = 1,$$

and it can be shown that for a many-electron atom the sum of the oscillator strengths is equal to Z , the atomic number.

Wheeler & Bearden (1934) applied this sum rule to obtain the oscillator strengths without the extrapolation of the continuum of the hydrogen-like atom used in the Hönl method. Recall, from equation (4), that g_k is given by the integral of the oscillator density from ω_k to infinity, then this integral plus the transitions to all bound states is equal to unity by the sum rule. Therefore, for the K electrons,

$$g_K = 2\{1 - \sum_m g(K, m)\} \quad (10)$$

where $g(K, m)$ is the oscillator strength of the virtual oscillator associated with the transition from the state K to the state m . The sum has to be taken over the relatively few occupied states. For other edges, the factor 2 in equation (10) is replaced by the multiplicity of the initial state. Wheeler & Bearden (1934) applied this method to the K edge only and to only a few atoms, there being few wave functions available at that time. This method has apparently not been again used until the present.

Bethe (1930) has given expressions for the oscillator strengths of hydrogen-like atoms for transitions $nl \rightarrow n'l'$. These expressions depend on the energy difference and transition probability. The Hartree wave functions could be used directly with Bethe's formulae but it is in principle more accurate to correct the Hartree energy levels by applying spin and relativistic corrections. These corrections split the p , d , and f states into two levels characterized by the three quantum numbers nlj , with the new levels having multiplicities $(2j+1)$ where $j = l \pm \frac{1}{2}$.

Bethe's formulae for the oscillator strengths can no longer be used after the relativity and spin corrections have been applied. Dr James Young, of this Laboratory, has derived the expression for the oscillator strength of the transition from the state nlj to the state $n'l'j'$. Young's formula is given below.

$$g_{n'l'j'}^{n'lj} = \frac{1}{3} \Delta E \max(l, l') (2j' + 1) [W(l, j, l', j'; \frac{1}{2}, 1)]^2 \times F' \left[\int_0^\infty P_{n'l'}^* r P_{nl} dr \right]^2. \quad (11)$$

Here, the primes denote the final state, ΔE is the energy difference in Rydbergs between the initial

and final states, the factor $(2j'+1)$ gives the multiplicity of the final state, W is the Racah coefficient (Racah, 1942), F' is the fractional occupancy of the final state and P is r times the Hartree radial wave function. The integral is the coordinate matrix element $\langle n'l'|r|nl \rangle$ and its square is proportional to the probability of spontaneous transition from the state nl to the state $n'l'$.

When the relativistic wave functions described by Liberman, Waber & Cromer (1965) are used, the integral in equation (11) is replaced by

$$\int_0^\infty [A_{n'l'j'}^* r A_{n'l'j'} + (-1)^{l-l'+j-j'} B_{n'l'j'}^* r B_{n'l'j'}] dr \quad (12)$$

where A and B are, respectively, r times the major and minor components of the wave functions.

Initial calculations of oscillator strengths

The K oscillator strength for caesium was initially computed from the Hartree (H) wave functions, by using equations (10) and (11), in order to test the method and the computer program. The results essentially duplicated those of Wheeler & Bearden (1934). Spin and relativity corrections (Slater, 1960) were applied to the H eigenvalues. Differences between computed eigenvalues were used to obtain ΔE for use in (11) rather than using experimental values of ΔE . This was done for convenience and also because experimental values of ΔE are not available for all transitions of interest for all elements.

More extensive oscillator strength calculations were then made for wolfram and uranium. The results for these heavy atoms did not agree well with Hönl's (1933) values and it was clear that the H wave functions were inadequate for this purpose. Relativistic Hartree-Dirac (HD) wave functions without exchange were available for wolfram and uranium (Cohen, 1960). The calculations were repeated with these wave functions and the results were considerably improved.

As an example, values of the individual terms used to calculate the oscillator strengths of the four innermost absorption edges of uranium are given in Table 1. The values from the H, the HD and the DS wave functions (DS wave functions were finally used for all atoms) are given so that the effect of better approximations to the true wave functions can be seen. The energy differences in Table 1 are given in terms of wavelength. The Hartree ΔE values for many transitions differ appreciably from experimental values but it can be seen that this error is minor as compared with the error in the transition probabilities computed from these wave functions.

Table 2 lists, for wolfram and uranium, the oscillator strengths calculated from the three different wave functions. Hönl's (1933) values are also listed for comparison.

Oscillator strengths and dispersion terms for elements 10 through 98

At this stage of the investigation the DS wave functions became available for all the atoms. Oscillator strengths were computed for elements 10 through 98 and these values are listed in Table 3. For elements 10 through 17, four absorption edges were considered; for elements 18 through 28, seven edges; elements 30 through 54, nine edges; elements 55 through 70, fourteen edges and for elements 71 through 98, sixteen edges were considered. Note that for neon and argon, for which the total number of electrons in the atoms is included in the edges considered, the sum of the oscillator strengths equals the number of electrons; thus the sum rule is satisfied.

The dispersion terms $\Delta f'$ were then computed by using Parratt & Hempstead's (1954) solution of equation (8) and summing over the various edges considered. For all atoms, $n=11/4$ was used for the $1s_{1/2}$ edge, $n=7/3$ for the $2s_{1/2}$ edge and for all other edges, $n=5/2$ was used. These are the same values of n used by Dauben & Templeton (1955). The dispersion terms $\Delta f''$ were computed from equation (9), again by summing over the various edges. Calculations were made for five different radiations in relatively common use. The results of these calculations are given in Table 4. Values are given only for $\sin \theta/\lambda=0$. Although the dispersion terms are functions of $\sin \theta/\lambda$, the variation is so small that it can be neglected in most crystal structure work.

The values of ω_k , the frequencies of the various absorption edges used in equations (8) and (9), were for the most part taken from the tabulation of energy levels by Sandström (1957). Where Sandström does not list energy levels, computed eigenvalues were used for ω_k . The asterisk after an element in Table 4 indicates that one or more computed eigenvalues were used in the calculations. Table 5 gives the computed eigenvalues that were used.

These dispersion terms are, in general, not much different from those calculated by Dauben & Templeton (1955), because the oscillator strengths used here are not much different from those previously determined by other methods. However, the dispersion terms given here are probably as accurate as can be computed by the present theoretical methods, because reasonably accurate oscillator strengths have been

used and because the contributions of the various absorption edges have been individually considered. More accurate wave functions, such as relativistic Hartree-Fock wave functions or those wave functions with correlation effects included, would probably not change the oscillator strengths very much.

The main limitations on the accuracy of these calculations are the uncertainty in the value of n in equations (8) and (9) and, more fundamentally, the questionable validity of equation (6), in which the exponential factor n is introduced. Also, for incident frequencies near an absorption edge, the exact position of the edge becomes of primary importance.

Sufficient information is given in Tables 3 and 5 so that one can compute the dispersion terms for other radiations or with other values of n for any atom.

I wish to thank Dr James Young and Dr James Waber for many helpful discussions.

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