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Calculation of the total Rayleigh scattering cross sections of photons in the energy range of 30–50 keV for Nb and Mo elements

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ABSTRACT

The total Rayleigh scattering cross sections are calculated in the energy range of 30–50 keV using the modified relativistic form factors (MRFF), non-relativistic form factors (NFF), and relativistic form factors (RFF). Numerical calculations are made for energies above the *K*-threshold comparisons, for medium-*Z* elements (Nb and Mo), primarily at small momentum transfers. The integration range is divided into intervals using a modified formula to take into account the smaller scattering angles. The calculated cross sections based on MRFF, NFF, and RFF are presented and compared with the tabulated theoretical values. It is found that the values calculated using the NFF and RFF are smaller than the tabulated values with a ratio of 3–7%. It is also observed that the smallest total Rayleigh scattering cross section values are obtained using the MRFF.

1. Introduction

Elastic scattering of photons by atoms, ions, or molecules is important in many fields such as crystallography, plasma physics, and astrophysics. Elastic scattering, in addition to its applications in shielding and in medical diagnostics, is used extensively to obtain information about the structural properties of materials and complex molecules (Roy et al., 1999). The elastic scattering of gamma rays by atoms occurs mainly through the coherent contributions of the following component processes that are Rayleigh scattering, nuclear Thomson scattering, Delbrück scattering, and nuclear resonance scattering. In Rayleigh scattering, photons are scattered by bound electrons in a process in which the atom is neither ionized nor excited. The photon loses only a negligible fraction of its energy, since the recoil is by the entire atom including the nucleus, rather than by an individual atomic electron as in the Compton effect (Hubbell, 1999, 2006). For the low energy region below 100 keV, the Rayleigh scattering is significantly the sole component of the elastic scattering (Kissel, 2000; Kissel et al., 1980). For the intermediate energy range of 0.1–2 MeV, the Rayleigh amplitudes dominate the elastic scattering amplitude for most scattering angles, and the photon energy is typically large compared with electron binding energy (Kissel, 2000; Kissel et al., 1980). For photon energies greater than about 2 MeV, the Rayleigh scattering is dominant only for very small scattering angles (Kissel et al., 1980). The nuclear Thomson scattering is important in the 100 keV and higher energies for high-*Z* atoms at medium and low angles (Kissel, 2000). Delbrück scattering contributions were shown to be negligible below about 0.662 MeV in several studies (Kane, 2005). Nuclear resonance scattering is expected to contribute to the total scattering for photon energies higher than about 1 MeV (Kissel, 2000).

Current theoretical efforts towards improved values of the coherent scattering cross section are focused on the second-order relativistic S-matrix approach (Kissel, 1995; Kissel et al., 1980; Pratt et al., 1994). In addition to the S-matrix values, this effort has generated systematic tabulations of related quantities that are of interest for scattering and other investigations. These quantities include self-consistent atomic potentials, form-factors, anomalous scattering factors (ASF), and bound–bound oscillator strengths. These values and selected programs have been collected in the form of a database that is called RTAB (Kissel, 2000). Extensive tabulations of the differential elastic scattering cross sections for all atoms for photon energies 0.0543–2754.1 keV available via the world wide web (www) at, http://adg.llnl.gov/Research/scattering/RTAB.html.

The National Institute of Standards and Technology (NIST) maintains a large number of database; several of these deal directly with photon–atom interactions. Most closely related to the information contained in this study are NIST form factors, attenuation and scattering tables, NIST X-ray, gamma-ray attenuation coefficients, and cross section database. Extensive calculations and theoretical tabulations of form factors, scattering cross sections, and quantities related to μ/ρ developed by Chantler (1995, 2000) are available in NIST on-line, http://www.nist.gov/pml/data/ffast/index.cfm.

International Tables for Crystallography is the definitive resource and reference work for crystallography. A detailed description of the theoretical and experimental techniques for the determination of X-ray absorption (and attenuation coefficients) is given by

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Arndt et al. (2006). An artificial distinction is made between the relativistic Dirac–Hartree–Fock–Slater (RDHFS) formalism used to calculate the data in these tables and the S-matrix method. Comparison with experimental data is showed to give a better fit to experimental results of the RDHFS formalism (Arndth et al., 2006). Further information can be found at the web page of http://it.iucr.org/Cb/ch4o2v0001/contents/.

Comparison of experimental results with different theories for different photon energies and targets are presented (Roy et al., 1993). As can be seen, MRFF with angle independent anomalous scattering factor improves agreement with experiments for all angles and photon energies near and below *K*-threshold, while predicted values using S-matrix agree quite well with experimental results. It can be seen that for all elements FF approximation gives, in general, good predictions for photon energies well above *K*-threshold, but it produces extremely poor results for photon energies close and below the *K*-threshold (Roy et al., 1993). Experimental results are also compared with theoretical estimates by Rao et al. (2002). It was shown that the values based on S-matrix and MRFF–ASF approaches are in excellent agreement with experimental results in the studied energy and atomic region. However, fairly good correspondence is observed between the experimental results and the values based on RFF–ASF approach compared to RFF and MRFF values (Rao et al., 2002).

The form-factor (FF) approximation, often used to predict Rayleigh scattering amplitudes, is believed to be accurate for small momentum transfers when the photon energy is large compared to binding energies of all the atomic electrons (Bradley et al., 1999b; Kissel et al., 1980; Roy et al., 1983). At the photon energies below 100 keV, experimental measurements have been compared with the form-factor approximation and reported theoretical predictions in good agreement with experiments (Kissel et al., 1980).

At the photon energies below 50 keV, the differential Rayleigh scattering cross sections were computed by Bradley et al. (1999b) using angle-independent anomalous scattering factors and MRFF for 1.486, 2.622, 4.086, 5.415, 8.048, 17.48, and 22.16 keV energies for biomedically important elements. The total Rayleigh scattering cross section was also calculated by Kissel et al. (1980) using the relativistic S-matrix values for 22.1 keV photon energy and lead ($Z=82$) element. Apart from these studies, as far as it is known by now, there has not been any theoretical prediction on the total Rayleigh scattering cross sections for the photon energies lower than 50 keV using the MRFF. Therefore, this work is focused on the calculation of the total Rayleigh scattering cross sections for small momentum transfers and selected two elements (Nb and Mo), and photon energies in the range of 30–50 keV. Theoretical predictions of form factors are based on MRFF (Schaupp et al., 1983), NFF (Hubbell et al., 1975), and RFF (Hubbell and Øverbø, 1979) versions. The theoretical predictions that are calculated by using the NFF and RFF are compared with the predictions of Hubbell et al. (1975) and Hubbell and Øverbø (1979) and seen to be lower with a ratio of 3–7%. It is also observed that the theoretical calculations based on MRFF are smaller than those based on NFF and RFF.

2. Form-factor approximations

The FF approximations are widely used and at least successful, in estimating the scattering cross sections. The atomic form factor could be derived both classically and quantum mechanically. It is defined for a spherically symmetric charge number density and momentum transfer. The FF approximation provides binding correction to the Thomson cross section and describes classical scattering from an electron charge distribution as a sum of subshell charge distributions rather than from a point charge. The FF approximation breaks down badly when the photon energy is near or below the inner shell photoeffect thresholds, or at large momentum transfers (large scattering angles and high photon energy; Bradley et al., 1999b; Kissel et al., 1980). It has been found to be useful for the description of Rayleigh scattering, especially for small momentum transfers and photon energies much larger than *K*-shell electron binding energies (Basavaraju et al., 1994; Kissel, 2000).

Brown and Mayers (1957) have proposed to use the MRFF approximation to the FF approximation, which was originally suggested by Franz (1935,1936). The accuracy of MRFF is studied by Kissel et al. (1980). The MRFF has a further electron-binding correction, resulting in substantially improved high energy limit values compared with the form factor, particularly in high-*Z* elements (Bradley et al., 1999b). The MRFF approximation gives the atomic Rayleigh scattering amplitudes with good accuracy for photon energies above *K*-shell binding and small momentum transfers (Bradley et al., 1999b; Kissel and Pratt, 1978; Schaupp et al., 1983). Tabulations of modified relativistic atomic form factors have been presented for all neutral atoms by Schaupp et al. (1983).

In general, relativistic and non-relativistic form factors differ from each other by not more than a few percent when momentum transfer is not very large (Roy et al., 1999). It has been found (Roy et al., 1999) that the NFF, computed using non-relativistic wavefunctions, predicts differential cross section $d\sigma/d\Omega$ fairly well (within a few percent) for energies well above the *K*-shell photoeffect threshold in the forward direction for almost all elements. The differential cross section obtained in the NFF is good (errors less than about 10%) for all angles in light and medium elements and for small angles in heavy elements over a range of photon energies from somewhat above the *K*-shell photoeffect threshold to about ten times greater than this (Roy et al., 1999). Extensive tabulations of the non-relativistic and the relativistic form factors exist for all neutral atoms (Hubbell and Øverbø, 1979; Hubbell et al., 1975).

The MRFF and RFF have been independently evaluated in the RTAB database (Kissel, 2000). The MRFF values are found to agree closely with the values published by Schaupp et al. (1983). Similarly, the RFF values are found to agree closely with the values published by Hubbell and Øverbø (1979). Systematic tabulations of differential scattering cross sections in various approximations are being made available in the RTAB database. Some of these differential scattering tables are obtained using MRFF and RFF values of Kissel (2000), and also NFF values of Hubbell et al. (1975).

Above the *K*-shell photoeffect threshold, the errors in differential cross section predictions of MRFF for finite angles are about the same as those of NFF or RFF (Roy et al., 1999). The MRFF works very well for the total cross section for photon energies above the *K*-shell photoeffect threshold (Roy et al., 1999).

For a wide variation in atomic number, the MRFF theory of Rayleigh scattering has been shown to give a good account of the experimental data for $x<12$ Å^{-1} (İçelli and Erzeneoğlu, 2001; Kane, 2005; Kane et al., 1983).

3. Theoretical background

The theory of scattering of X-rays from free electrons was studied by J.J. Thomson, and it is called as the Thomson scattering. The unpolarized Thomson scattering cross section contains Rayleigh's result (Strutt, 1871a,b). Differential Thomson scattering cross section per electron, is given as

$$\frac{d\sigma^T}{d\Omega}=\frac{r_e^2}{2}(1+\cos^2\theta) \tag{1}$$

and the total, angle-integrated Thomson scattering cross section is

$$\sigma^T=\frac{8}{3}\pi r_e^2 \tag{2}$$

where the classical electron radius is $r_e=e^2/m_ec^2$.

The differential Rayleigh scattering cross section for elastic scattering of unpolarized photons through an angle θ, and averaged over scattered-photon polarizations in form-factor approximation may be written

$$\frac{d\sigma}{d\Omega} = \frac{r_e^2}{2}(1+\cos^2\theta)[F(x,Z)]^2 \quad (3)$$

The Rayleigh (coherent) scattering cross section per atom is given as

$$\sigma_{coh} = \int_{\theta=0}^{\theta=\pi} d\sigma^T(\theta)[F(x,Z)]^2 \quad (4)$$

One important feature to be noted (Roy et al., 1983) in all FF theories is that the term $(1+\cos^2\theta)/2$ resulting from the decision not to observe polarization may be factored out of the scattering cross section, yielding a reduced cross section.

The total Rayleigh (coherent) scattering cross sections are computed by using numerical integration of the Thomson (1906) formula weighted by $[F(x,Z)]^2$ defined in Eq. (4). The atomic form factor $F(x,Z)$ is a function of the variable x, which is $x=\lambda^{-1}\sin(\theta/2)$ (the momentum transfer variable dependent on the incident photon energy and the deflection angle of the scattered photon), and Z is the atomic number of the nucleus of the target atom.

4. Results and discussion

The total Rayleigh scattering (the sole component of elastic scattering in the present energy range) cross sections for medium-Z elements and for the photon energy range 30–50 keV have been calculated up to $x=5$ Å^{-1} using the MRFF, NFF, RFF approximations by numerically performing the integration defined in Eq. (4). These values are reported in Tables 1 and 2. The values of form factors at the integration mesh-points were obtained by an accurate interpolation from the tabulations widely used of Hubbell et al. (1975), Hubbell and Øverbø (1979), and Schaupp et al. (1983).

In calculations, the integration variable was taken as $1-\cos\theta$, from which the values of $x=\sin(\theta/2)/\lambda(\text{A}^\circ)=[(1-\cos\theta)/2]^{1/2}/\lambda(\text{A}^\circ)$ could be computed close to $\theta=0$. The integration range used, was from $1-\cos\theta=10^{-16}$ to 2.0 ($\theta=0.0000008538^\circ$–$180^\circ$), divided into intervals in the logarithm of $1-\cos\theta$ with the new formula developed in this study.

$$1-\cos\theta_i = \frac{a+(a/2^n-1)}{2^n}2^{i-1} \quad (5)$$

where, $a=2$ is the total integration range and i is the lower integration range varying from $i=1$ to n . In the studies of Hubbell et al. (1975) and Hubbell and Øverbø (1979), the integration range was taken from $1-\cos\theta=10^{-12}$ to 2.0. In this study, the integration range of $1-\cos\theta=10^{-16}$ to 2.0 was used since the smaller scattering angles were taken into account.

It has been shown by Bradley and Ghose (1986) that the differential Rayleigh scattering cross section values obtained by using the MRFF approximation are considerably smaller than the values obtained by applying the RFF and NFF approximations, and closer to the experimental data. It was mentioned (Bradley and Ghose, 1986; Bradley et al., 1999a; Kane, 2005; Kane et al.,1983) that the RFF approximation is seen to be inadequate for an explanation of experimental data while the MRFF approximation is better than RFF approximation and in agreement with experimental data, and the NFF approximation is closer to the experimental data than RFF calculations. It has been a general experience that the order of validity of form-factor approximations is MRFF, followed by NFF, with RFF yielding the poorest predictions.

In Tables 1 and 2, the smallest total Rayleigh scattering cross section values are obtained when the MRFF approximation of Schaupp et al. (1983) is used. This is followed by the NFF approximation of Hubbell et al. (1975) and then the RFF approximation of Hubbell and Øverbø (1979). On the other hand, the total scattering cross section values calculated by both using NFF (Hubbell et al., 1975) and RFF (Hubbell and Øverbø, 1979) approximations were found to be lower than the total scattering cross section predictions of Hubbell et al. (1975) and Hubbell and Øverbø (1979), with a ratio of 3–7%. This difference could be explained as a result of the calculations of the smaller scattering angles.

A major step in this effort is obtained from the work of Chatterjee and Roy (1998). They have presented the tables of differential and

Table 1
The calculated values of the total Rayleigh scattering cross sections for niobium (Nb-41) element obtained by using the MRFF, NFF, and RFF are presented in Columns 2, 3, and 4, respectively. The values of Hubbell et al. (1975) and Hubbell and Øverbø (1979) interpolated for the photon energies in this study can be seen in Columns 5 and 7, respectively. The differences between Columns 3 and 5 are presented in Column 6, and the differences between Columns 4 and 7 can be observed in Column 8.

E (keV)	Calculated cross sections (b/atom)			Hubbell et al. (1975)	% relative difference	Hubbell and Øverbø (1979)	% relative difference
	MRFF	NFF	RFF				
30	79.16	80.32	81.17	82.69	2.9	83.86	3.2
31	75.42	76.73	77.38	79.78	3.8	80.93	4.4
32	71.96	73.37	73.87	76.87	4.6	77.99	5.3
33	68.80	70.17	70.66	73.97	5.1	75.06	5.9
34	65.78	67.10	67.59	71.06	5.6	72.13	6.3
35	63.00	64.17	64.75	68.15	5.8	69.19	6.4
36	60.37	61.42	62.07	65.24	5.9	66.26	6.3
37	57.88	59.00	59.52	62.33	5.3	63.33	6.0
38	55.58	56.66	57.18	59.43	4.7	60.40	5.3
39	53.39	54.38	54.94	56.52	3.8	57.46	4.4
40	51.28	52.15	52.79	53.61	2.7	54.53	3.2
41	49.35	50.13	50.82	51.99	3.6	52.88	3.9
42	47.52	48.29	48.96	50.36	4.1	51.24	4.5
43	45.74	46.50	47.14	48.74	4.6	49.59	4.9
44	44.07	44.92	45.43	47.12	4.7	47.95	5.3
45	42.48	43.37	43.81	45.49	4.7	46.30	5.4
46	40.98	41.85	42.27	43.87	4.6	44.65	5.3
47	39.57	40.41	40.83	42.25	4.4	43.01	5.1
48	38.20	39.00	39.42	40.63	4.0	41.36	4.7
49	36.90	37.64	38.10	39.00	3.5	39.72	4.1
50	35.69	36.32	36.85	37.38	2.8	38.07	3.2

Table 2
The calculated values of the total Rayleigh scattering cross sections for molybdenum (Mo-42) element obtained by using the MRFF, NFF, and RFF are presented in Columns 2, 3, and 4, respectively. The values of Hubbell et al. (1975) and Hubbell and Øverbø (1979) interpolated for the photon energies in this study can be seen in Columns 5 and 7, respectively. The differences between Columns 3 and 5 are presented in Column 6, and the differences between Columns 4 and 7 can be observed in Column 8.

E (keV)	Calculated cross sections (b/atom)			Hubbell et al. (1975)	% relative difference	Hubbell and Øverbø (1979)	% relative difference
	MRFF	NFF	RFF				
30	83.80	85.03	86.09	87.57	2.9	88.95	3.2
31	79.86	81.24	82.07	84.50	3.9	85.85	4.4
32	76.20	77.70	78.34	81.43	4.6	82.75	5.3
33	72.86	74.33	74.94	78.35	5.1	79.64	5.9
34	69.68	71.10	71.69	75.28	5.5	76.54	6.3
35	66.73	68.01	68.69	72.21	5.8	73.44	6.5
36	63.96	65.11	65.86	69.14	5.8	70.34	6.4
37	61.33	62.55	63.18	66.07	5.3	67.24	6.0
38	58.91	60.07	60.70	62.99	4.6	64.13	5.3
39	56.60	57.65	58.34	59.92	3.8	61.03	4.4
40	54.37	55.28	56.07	56.85	2.8	57.93	3.2
41	52.34	53.15	53.99	55.14	3.6	56.19	3.9
42	50.42	51.21	52.03	53.42	4.1	54.45	4.4
43	48.55	49.32	50.11	51.71	4.6	52.71	4.9
44	46.79	47.66	48.31	49.99	4.7	50.97	5.2
45	45.11	46.03	46.59	48.28	4.7	49.23	5.4
46	43.53	44.44	44.97	46.57	4.6	47.49	5.3
47	42.03	42.92	43.44	44.85	4.3	45.75	5.0
48	40.59	41.44	41.95	43.14	3.9	44.01	4.7
49	39.22	40.00	40.55	41.42	3.4	42.27	4.1
50	37.93	38.62	39.23	39.71	2.7	40.53	3.2

total elastic scattering cross sections in the atomic number range $Z=13$–104 for photon energies in the range 50–1500 keV using the NFF, RFF approximations, and S-matrix values. However, the tables in this study consist of the total Rayleigh scattering cross sections for photon energies in the range of 30–50 keV, and for Nb and Mo elements using the MRFF, NFF, and RFF approximations.

It has been established both from experiments and from the comparison with S-matrix results that MRFF, in general, produces better results than other choices of form factors (Kissel, 2000; Roy et al., 1993). Like the FF approximation, the MRFF approximation breaks down badly when the photon energy is near or below the photoeffect thresholds or at large momentum transfers (Bradley et al., 1999b). The MRFF approximation gives good predictions for all elements for zero-angle scattering for photon energies well above K-shell binding (Bradley et al., 1999b; Roy et al., 1993, 1999; Zhou and Pratt, 1990). Dispersion corrections to form factor amplitudes or the so-called anomalous scattering factors (Cromer, 1983; Cromer and Liberman, 1970) are shown (Kane, 2005) to be needed at photon energies close to electron binding energy thresholds.

It can be concluded that the MRFF theory seems to be an approximation, which is better than NFF and RFF theories for energies above the K-threshold comparisons. The total Rayleigh scattering cross sections based on MRFF can be used to assist the experimental findings. Furthermore, these values can be interpolated to determine the cross sections for any other energies in the energy range of 30–50 keV.

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