The Effect of Electron Incident Energy on Total Cross Section Calculations for the Noble Gases

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ABSTRACT

Calculated Total Cross-Sections (TCS) of elastic electron-atom scattering for the noble gases He, Ne, Ar, Kr, Xe and Rn are presented. The computed TCS were calculated using the partial wave, Eikonal, Born, and the optical theorem approximation methods with the Lenz-Jensen potential, at electron incident energies between 1to1000 eV. Results obtained using the partial wave, Eikonal and optical theorem approximation methods are in good agreement with experimental TCS data.

Keywords: Total Cross-Sections, elastic scattering, noble gases, partial wave, Eikonal, optical theorem, Born approximation.

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INTRODUCTION

In scattering theory, the Total Cross-Section (TCS) is a measure of the probability that an interaction occurs; the larger the cross section, the greater the probability that an interaction will take place when a particle is incident on a target [1].

Elastic electron-atom scattering takes place if the final state of an atom after the interaction coincides with the initial one [2]. Total and differential cross-sections for such a process can be calculated in various approximations — Born [3], Eikonal [4,5], optical theorem [6,7] partial wave method [8] etc. In this work, the total cross-sections of the noble gases He, Ne, Ar, Kr, Xe and Rn [9,10] were computed using the four approximation methods listed above.

MATERIALS AND METHODS

We used the FORTRAN code program developed by [11] which takes the relativistic differential cross-section as a sum of squared modules of the real and imaginary scattering amplitudes. The amplitudes can be calculated through the phase shifts of spherical waves, which are obtained by integration of equations for radial wave functions. In these computations the analytical approximation for the atomic electrostatic potential given by Lenz and Jensen, called the Lenz-Jensen potential [12], based on the Thomas-Fermi model, is used.

Scattering Theory

For particles of mass m and energy

$$E = \frac{\hbar^2 k^2}{2m} > 0 \qquad 1.0$$

scattering from a central potential, V(r) is described by a wave function, ψ(r) that satisfies the Schrodinger Wave Equation (SWE)

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \qquad 2.0$$

with the boundary condition at large distance

$$\psi_{r\to\infty} \to e^{ikz} + f(\theta)\frac{e^{ikr}}{r} \qquad 3.0$$

Equation (3.0) holds for a beam of electrons incident along z-axis, and the scattering angle, θ is the angle between r and $\hat{z}$ while f is the complex scattering amplitude, which is the basic function we seek to determine. The differential cross-section is given by:

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 \qquad 4.0$$

The total cross-section is

$$\sigma = \int d\Omega \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = 2\pi \int_0^{\pi} \mathrm{d}\theta \sin\theta |\mathrm{f}(\theta)|^2 \qquad 5.0$$

f is a function of both E and θ [11].

Approximation Methods

Approximations play a very important role in our understanding of processes that cannot be solved exactly. The calculation of scattering cross sections is one of the most important uses of Fermi's Golden Rule [13]. Fermi's rule involves only one matrix element of the interaction which makes it a first order approximation to the

exact result. This approximation suggests an approximation to the complex scattering amplitude.

The Born approximation involves an approximation to the complex scattering amplitude [3]. It has been extensively used to study low energy as well as high energy scattering processes. The Eikonal approximation is a technique for estimating the high energy behaviour of a forward scattering amplitude [4]. It was originally developed for potential scattering in quantum mechanics, where one approximates the classical trajectory corresponding to forward scattering by a straight line and uses a WKB approximation for the wavefunction [14]. The optical theorem relates the forward scattering amplitude to the cross section [6].

Partial Wave Method

The method of partial wave expansion is a special trick to simplify the calculation of the scattering amplitude, f [15]. The standard partial wave decomposition of the scattering wave function ψ is

$$\psi(r) = \sum_{l=0}^{\infty}(2l+1)i^l e^{i\sigma}\frac{R_l(r)}{kr}P_l(cos\theta) \qquad 6.0$$

When equation (2.6) is substituted into the SWE (2.0) the radial wave functions, R_l are found to satisfy the radial differential equations:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) + \frac{l(l+1)\hbar^2}{2mr^2} - E\right]R_l(r) = 0 \qquad 7.0$$

This is the same equation as that satisfied by a bound state wave function but the boundary conditions are different. In particular, R vanishes at the origin, but it has the large-r asymptotic behaviour

$$R_l \to kr[cos\delta_l j_l(kr) - sin\delta_l n_l(kr)] \quad 8.0$$

Where j_l and n_l are the regular and irregular spherical Bessel functions of order l. The scattering amplitude is related to the phase shifts δ_l by [9]:

$$f(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}sin\delta_l P_l(cos\theta) \quad 9.0$$

From equations (5.0) and (9.0) the total cross-section is given by

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)sin^2\delta_l \quad 10.0$$

Although the sums in equations (9.0) and (10.0) extend over all l, they are in practice limited to only a finite number of partial waves. This is because for large l, the repulsive centrifugal potential in equation (7.0) is effective in keeping the particle outside the range of the potential and so the phase shift is very small.

If the potential is negligible beyond a radius r_{max}, an estimate of the highest partial wave that is important is had by setting the turning point at this radius:

$$\frac{l_{max}(l_{max}+1)\hbar^2}{2mr_{max}^2} = E \quad 11.0$$

$$\Rightarrow \quad l_{max} \approx kr_{max} \quad 12.0$$

This estimate is usually slightly low since the penetration of the centrifugal barrier leads to non-vanishing phase shifts in partial waves somewhat higher than this (Koonin & Meredith, 1989).

The Phase shifts

To find the phase shift in a given partial wave, we must solve the radial equation (7.0). The equation is linear, so that the boundary condition at large r can be satisfied simply by appropriately normalizing the solution.

If we put $R_l(r=0)=0$ and take the value at the next lattice point, $R_l(r=h)$, to be any convenient small number we then use

$$f^{"} \approx \frac{f_1-2f_0+f_{-1}}{h^2} \qquad 13.0$$

for $R_l^{"}(h)$, along with the known values $R_l(0)$, $R_l(h)$, and $k(h)$ to find $R_l(2h)$. Now we can integrate outward in r to a radius $r^{(1)} > r_{max}$. Here, V vanishes and R must be a linear combination of the free solutions, $krj_l(kr)$ and $krn_l(kr)$:

$$R_l^{(1)} = Akr^{(1)}\left[cos\delta_l j_l\left(kr^{(1)}\right) - sin\delta_l n_l\left(kr^{(1)}\right)\right] \qquad 14.0$$

Although the constant, A above, depends on the value chosen for $R(r=h)$, it is largely irrelevant for our purposes; however, it must be kept small enough so that overflows are avoided. Now we continue integrating to a larger radius $r^{(2)} > r^{(1)}$:

$$R_l^{(2)} = Akr^{(2)}\left[cos\delta_l j_l\left(kr^{(2)}\right) - sin\delta_l n_l\left(kr^{(2)}\right)\right] \qquad 15.0$$

Equations (14.0) and (15.0) can then be solved for δ_l to obtain

$$tan\delta_l = \frac{G j_l^{(1)} - j_l^{(2)}}{G n_l^{(1)} - n_l^{(2)}};\ G = \frac{r^{(1)} R_l^{(2)}}{r^{(2)} R_l^{(1)}} \qquad 16.0$$

where $j_l^{(1)} = j_l(kr^{(1)}$ etc. Equation (16.0) determines δ_l only within a multiple of π but this does not affect the physical observables [see equations (9.0) and (10.0)].

The correct multiple of π's at a given energy can be determined by comparing the number of nodes in R and in the free solution, krj_l which occur for $r < r_{max}$. The phase shift in each partial wave vanishes at high energies and approaches $N_l\pi$ at zero energy, where N_l is the number of bound states in the potential in the l'th partial wave [11].

The Lenz-Jensen Potential

One practical application of the theory discussed above is the calculation of the scattering of electrons from neutral atoms. In general this is a complicated multi-channel scattering problem since there can be reactions leading to final states in which the atom is excited. However, as the reaction probabilities are small in comparison to elastic scattering, for many purposes the problem can be modeled by the scattering of an electron from a central potential [11]. This potential represents the combined influence of the attraction of the central nuclear charge (Z) and the screening of this attraction by the Z atomic electrons. For a neutral target atom, the potential vanishes at large distances faster than r^{-1}**.** A very accurate approximation to this potential can be had by solving for the self-consistent Hartree-Fock potential of the neutral atom. However, a much simpler estimate can be obtained using an approximation to the Thomas-Fermi model of the atom given by Lenz and Jensen [12].

$$V = -\frac{Ze^2}{r}e^{-x}(1 + x + b_2x^2 + b_3x^3 + b_4x^4); \qquad 17.0$$

with

$$e^2 = 14.409;\ b_2 = 0.3344;\ b_3 = 0.0485;\ b_4 = 2.647 \times 10^{-3}; \qquad 18.0$$

and

$$x = 4.5397 Z^{\frac{1}{6}} r^{\frac{1}{2}} \qquad 19.0$$

This potential is singular at the origin. If the potential is regularized by taking it to be a constant within some small radius r_{min} (say the radius of the atom's 1s shell), then the calculated cross-section will be unaffected except at momentum transfers large enough so that $qr_{min} \gg 1$. The incident particle is assumed to have the mass of the electron, and, as is appropriate for atomic systems, all lengths are measured in angstrom (Å) and all energies in electronvolt (eV). The potential is assumed to vanish beyond 2Å. Furthermore, the r^{-1} singularity in the potential is cutoff inside the radius of the 1s shell of the target atom.

The Noble Gases

The noble gases helium (He), neon (Ne), argon (Ar), krypton (Kr), xenon (Xe), and radon (Rn) were discovered during the 1800s. Helium has two electrons; neon has ten; argon has eighteen; krypton has thirty-six; xenon has fifty-four; and radon has eighty-six. All of the noble gases exist on Earth as products of radioactive decay of other elements [9]. The noble gases exist in the atmosphere only as monatomic gases; that is, a noble gas molecule consists of a single atom rather than two atoms like N_2 and O_2.

The chemical inertness of the noble gases is attributed to their electronic configurations. The lightest noble gas, helium, has a configuration of $1s^2$, which means its only two electrons are in a filled energy level, and helium does not form chemical bonds. The remaining noble gases have configurations that end in the pattern ns^2np^6, where n is the energy level. These configurations are:

Ne - [He] $2s^2 2p^6$

Ar - [Ne] $3s^2 3p^6$

Kr - [Ar] $3d^{10} 4s^2 4p^6$

Xe - [Kr] $4d^{10} 5s^2 5p^6$

Rn - [Xe] $4f^{14} 5d^{10} 6s^2 6p^6$.

In 1962, Neil Bartlett, a Canadian chemist at the University of British Columbia, made XeF_2 by combining xenon gas with fluorine gas in the presence of sunlight [9]. He, along with other scientists around the world, subsequently succeeded in making other compounds of xenon and krypton—mostly fluorides, oxides, and oxyfluorides. To date, however, no compounds have been made with helium, neon, or argon [9].

Research Methodology

A FORTRAN program developed by [11] was the main program used for all the computations. The program is made up of four categories of files: common utility programs, physics source code, data files and include files. The physics source code is the main source code which contains the routine for the actual computations. The data files contain data to be read into the main program at run-time and have the extension .DAT The first thing done was the successful installation of the FORTRAN codes in the computer. This requires familiarity with the computer's operating system, the FORTRAN compiler, linker, editor, and the graphics package to be used in plotting. The program runs interactively. It begins with a title page describing the physical problem to be investigated and the output that will be produced. Next, the menu is displayed, giving the choice of entering

parameter values, examining parameter values, running the program, or terminating the program. When the calculation is finished, all values are zeroed (except default parameters), and the main menu is re-displayed, giving us the opportunity to redo the calculation with a new set of parameters or to end execution. Data generated from the program were saved in files which were later imported into the graphics software *Origin 5.0* for plotting.

RESULTS

Results were generated for several electron incident energies and the graphics software *Origin 5.0* used to plot graphs.

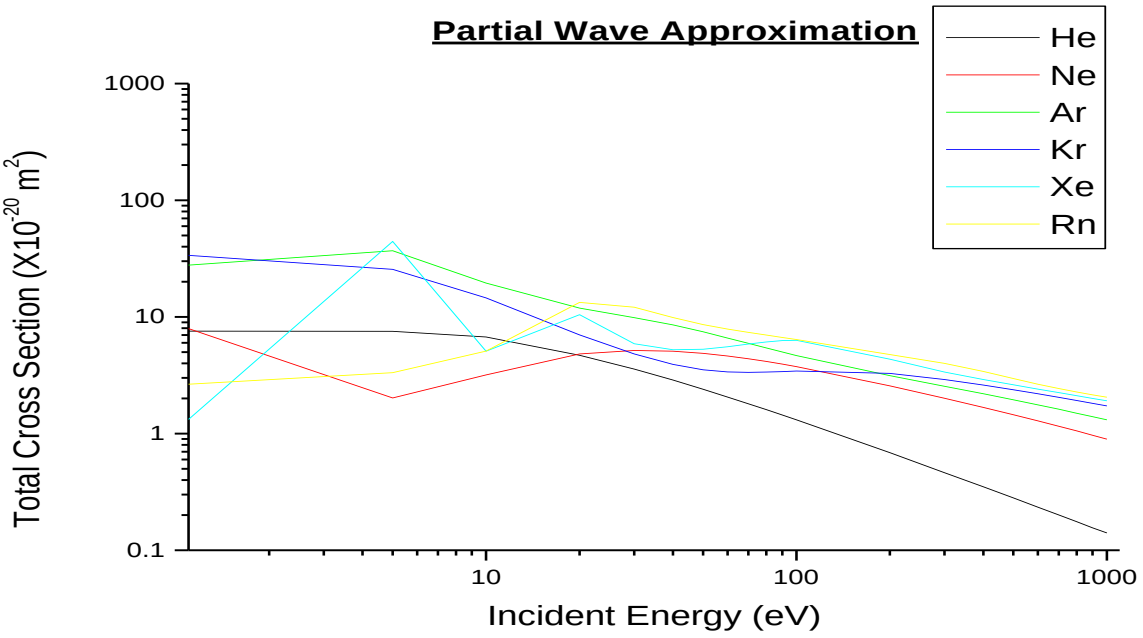

Fig. 1: Comparisons of the energy dependence of the Total Cross-Sections of He, Ne, Ar, Kr, Xe and Rn using the Partial Wave Decomposition method.

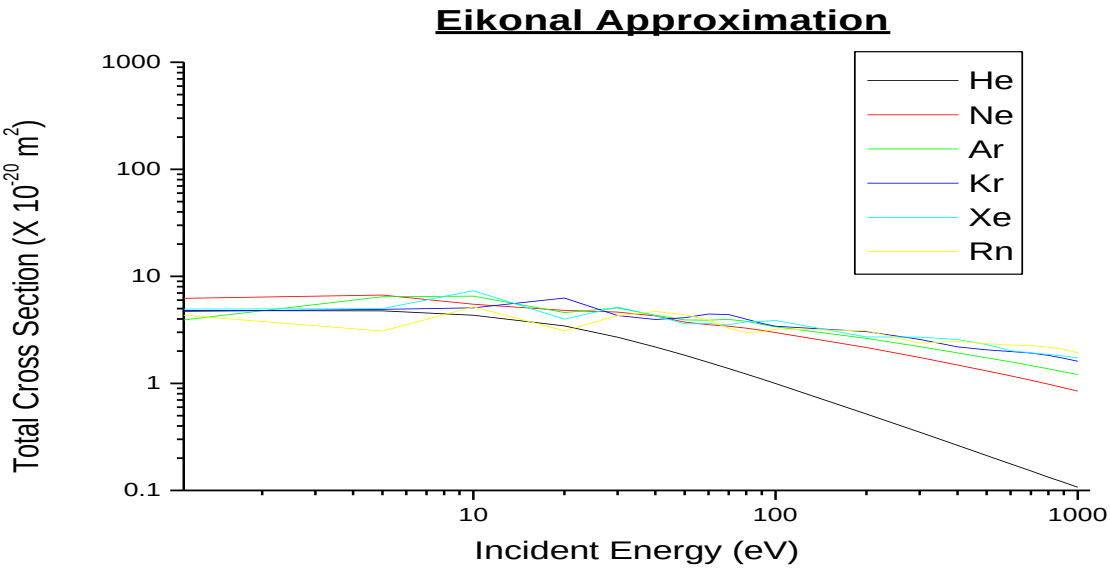

Fig. 2: Comparisons of the energy dependence of the Total Cross-Sections of He, Ne, Ar, Kr, Xe and Rn using the Eikonal approximation method.

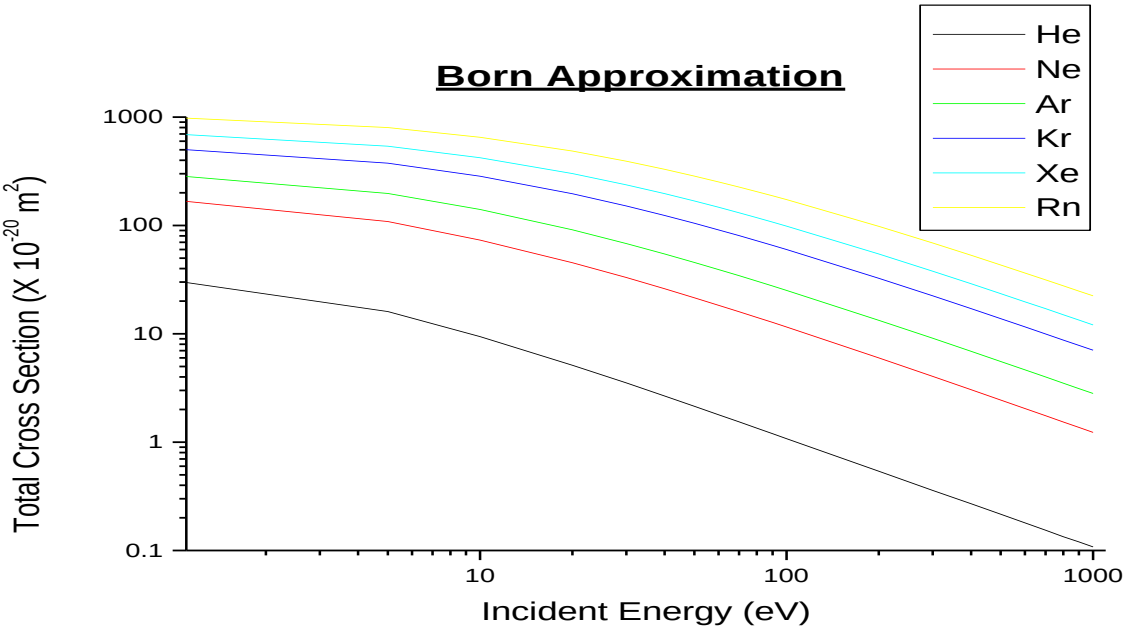

Fig. 3: Comparisons of the energy dependence of the Total Cross-Sections of He, Ne, Ar, Kr, Xe and Rn using the Born approximation method.

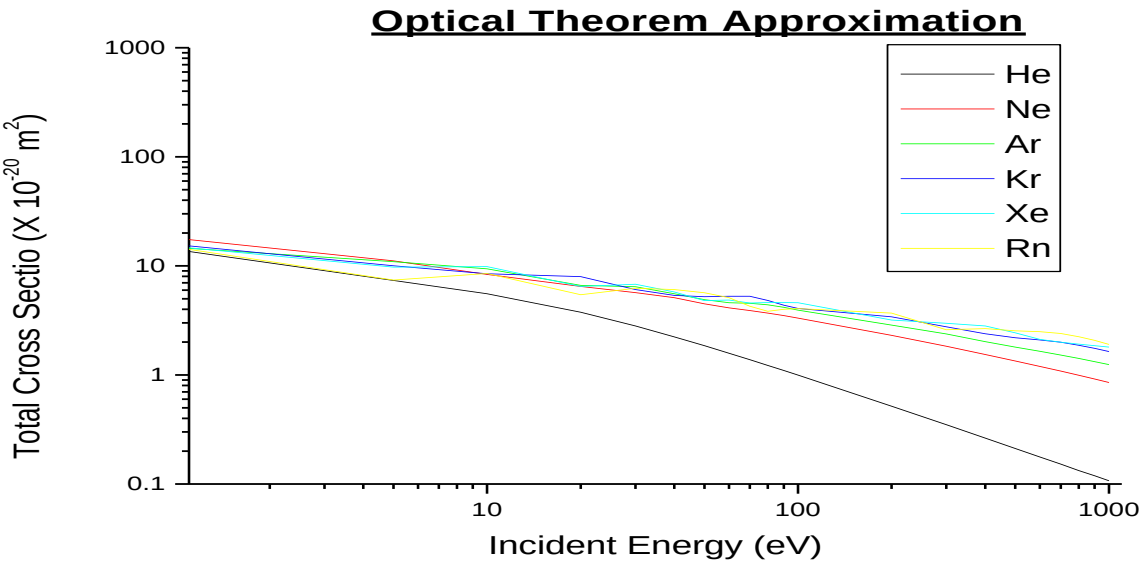

Fig. 4: Comparisons of the energy dependence of the Total Cross-Sections of He, Ne, Ar, Kr, Xe and Rn using the Optical Theorem approximation method.

DISCUSSION

The total cross-sections computed using the partial wave decomposition method have inverse relationships with the electron incident energies. This is in agreement with theoretical data of [16] and experimental data of [10]. Total cross-section data obtained using the partial wave method are in good agreement with data from National Institute of Standards and Technology (NIST) Standard Reference Database 64 (SRD 64). Data from Eikonal approximation method are in good agreement with present work but lower. However, data from the Born approximation method disagree widely with present work, Eikonal and NIST SRD 64 data at low incident energies. These disagreements were anticipated as the Born approximation is valid only at high electron incident energies. However, there is good agreement between the Born and other approximation methods at high incident energies as expected.

From fig. 1 above, using the partial wave method, we observed that the TCS for He decrease with increasing electron incident energies from 1 to 1,000 eV. The TCS for Ne, Ar, Xe and Rn exhibited a number of minima and maxima between 1 to 100 eV, but decrease with increasing incident energies between 100 to 1,000 eV. Also, the TCS increase with increasing atomic number for the noble gases. The differences in TCS for He, in the energy range of about 70 to 1,000 eV, are substantially higher than differences in TCS for other noble gases. This might have resulted from the fact that He has an "S" valance shell while all the others have "P" valence shells.

From fig. 2, using the Eikonal method, the TCS for He also decrease with increasing electron incident energies from 1 to 1,000 eV. The TCS for Ne, Ar, kr, Xe and Rn exhibited a number of minima and maxima between 1 to 30 eV, but decrease with increasing incident energies between 30 to 1,000 eV. Also, the TCS increase with increasing atomic number for the noble gases. The differences in TCS for He, in the energy range of about 50 to 1,000 eV, are substantially higher than differences in TCS for other noble gases.

From fig. 3, using the Born method, the calculated TCS are significantly higher than the TCS obtained using the three other approximation methods. This is as a result of the fact that the Born approximation is only valid at high electron incident energies. As previously observed, the calculated TCS decrease with increasing incident energies but no minima and maxima were observed for all the noble gases.

From fig. 4, using the optical theorem method, the calculated TCS for Kr, Xe and Rn exhibited a number of minima and maxima in the energy range of 1 to 100 eV. No minima or maxima were observed for He, Ne and Ar. Here also, the calculated TCS decrease with increasing electron incident energies.

The calculated TCS using the partial wave, Eikonal and optical theorem approximation methods are generally in good agreement with the experimental TCS obtained by [16]. However TCS calculated using the Born approximation method are much higher than the experimental values for the energy range considered. This is because the Born approximation is only valid at high electron incident energies.

CONCLUSION

Computed Total Cross-Sections (TCS) of elastic electron-atom scattering for the noble gases He, Ne, Ar, Kr, Xe and Rn are presented. The TCS were calculated using the partial wave, Eikonal, Born, and the optical theorem approximation methods with the Lenz-Jensen potential, at incident energies of 1to1000 eV. Results obtained using the partial wave, Eikonal and optical theorem methods are in good agreement with the experimental TCS values reported by [16].

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