Advances in Physics Theories and Applications
ISSN 2224-719X (Paper) ISSN 2225-0638 (Online)
Vol.54, 2016

Total Electron Scattering Cross Section by Diatomic Molecules

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Abstract
Total scattering cross section of electron scattering by diatomic molecule is studied theoretically. Total scattering cross section of electron scattering by diatomic molecule has been calculated via Born Approximation. Model for electron scattering by diatomic H_2, S_2, and O_2 are made. Calculation result is then compared with previously published experimental values by Brunger and Buckman (2002), Naghma et al (2014). Scattering potential involved to represent diatomic molecule is Morse potential. The result shows that the total scattering cross section is decreasing as the incoming electron energy increasing. The calculated value is higher than experimental value. The result shows that below dissociation energy, 4.7 eV, calculated total scattering cross section is increasing as incoming electron energy increasing, might be due to recombination process and detector insensitivity for low energy electron, while for incoming electron energy higher than 4.7 eV, although calculated result gives higher value than experimental result, the experimental data shows similar trend to calculated model. Result is best for energies higher than 60 eV, although still higher than experimental data due to inelastic processes in experimental procedures. Building models for other diatomic molecules and making correction to low energy electron is suggested.
Keywords: electron scattering, diatomic molecule, Born approximation, Morse potential

1. Introduction

Scattering is one of the most important aspects in various fields of physics. The study of scattering becomes important in the development of instruments, such as *scanning electron microscope (SEM)* (Wight & Konicek 2012), in understanding the biological effect of radiation (Naghma et al 2014), and plasma development (Khamdani 2014). Electron scattering cross section by diatomic molecules understanding transport problem of particles in plasma as well as in ionic wind and Electrohydrodynamic (EHD) (Nur et. al., 2014a; Nur et. al. 2014b). Total scattering cross section shows the area of probable impact by the incoming particles and will be scattered to all direction. In other words, total scattering cross section shows the probability of collision between two particles. Unfortunately, theoretical approach in scattering theory has not shows satisfying result as proposed by Naghma et al (2014), Ariyasinghe et al.(2004), Moreh (2012), Tan and Wang (2011), and Wight & Konicek (2012).

The case of electron scattering by diatomic molecules can be reduced to a process of electron scattering due to the potential of diatomic molecules (Tannouji et al 1977). Various potentials are suggested to represent diatomic molecules, for instance Yukawa potential, both single and double (Liu & Sun 1996), Hulthen potential (Bayrak & Boztosun 2007), Morse potential (Bayrak & Boztosun 2007; Taseli 1998; Han et al 2005; Gronowski & Adamczak 2010; Roy 2013) and its derivatives such as Rosen-Morse potential (Amani 2015), *spherical complex optical potential (SCOP)*(Naghma et al 2014; Vinodkumar et al 2008). From those potentials, Morse potential is among the most frequently used to represent diatomic molecule behavior.

Various methods are used to solve for scattering cross section, such as independent atom method (IAM) (Mozejko & Szmytkowski 2003)

Born approximation has been used in calculation of scattering cross section for elastic collisions. Liu & Sun (1996) used Born approximation to find the formula of electron scattering cross section by diatomic molecule, using single and double Yukawa potential. Khamdani et al. (2014) used Born approximation for electron scattering cross section by ion. Ariyasinghe et al. (2004) combined Bethe theory and Born approximation to calculate electron scattering cross section by noble gases. Gronowski and Adamczak (2010) used Born approximation to calculate muonic particles scattering cross section by diatomic molecules in the atmosphere.

In this paper, total electron scattering cross section by diatomic molecules is studied theoretically using Born approximation and Morse potential serving as diatomic molecule potential.

2. Theory

For a target particle with potential *V(r),* the magnitude of scattering amplitude can be calculated using Born approximation. Standard formula for Born approximation is as follows (Liboff 2003)

$$f(\theta) = -\frac{2m}{\hbar^2 K}\int_0^\infty rV(r)\sin Krdr \tag{1}$$

where K is the difference between scattered and incoming wavenumber $K= k'-k$ and represents the change in wave vector prior to and after scattering process.
Morse potential is defined as follows

$$V_{Morse}(r) = D_e(e^{-2\alpha x} - 2e^{-\alpha x}) \tag{2}$$

where D_e is dissociation energy and $\alpha = ar_e$ is Morse parameter with r_e as the equilibrium distance (bond length) between constituting atoms inside the diatomic molecule and a is a parameter to control the width of *potential well*, while $x = (r-r_e)/r_e$.
Hence, equation (2) can also be written as

$$V(r) = D_e(e^{-2a(r-r_e)} - 2e^{-a(r-r_e)}) \tag{3}$$

Meanwhile the total scattering cross section can be calculated as follows (Liboff 2003)

$$\sigma = 2\pi\int_0^{\pi} |f(\theta)|^2 \sin\theta d\theta \tag{4}$$

3. Method

Total electron scattering cross section by diatomic molecule is studied theoretically. The potential used to represent diatomic molecule is Morse potential. Total scattering cross section is derived using Born approximation. Total scattering cross section is plotted against incoming electron energy for hydrogen H_2 molecules. The parameters used to model for hydrogen molecules is taken from Roy (2013), i.e.: dissociation energy of hydrogen molecule 4,7446 eV, reduced mass of hydrogen 0,50391 amu, Morse parameter for hydrogen α 1,440558, and the distance between constituting atom for hydrogen molecule r_e 0,7416 Å. Calculation result is then compared to experimental data by Brunger and Buckman (2002). This study is limited to elastic collision between electron and diatomic molecules with low to middle energy range. Born approximation is used in elastic scattering cases where the kinetic energy of the system does not change. In this case, no energy is absorbed by target particle so that the condition of target particle does not change. In this case, there is a number of assumption, i.e.: (1) the spin of the scattered particle and target particle is neglected, (2) the internal structure of particle is not taken into account, because incoming particle is seen as wave and target particle as potential, that means the scattering phenomenon will not change the internal structure of both scattered particle and target particle, (3) the size of target particle is very small so that we can assume multiple scattering will not occur, where incoming particle is scattering several times before it leaves the target particle,(4) the coherence between scattered wave by the structures that constitute the target particle can also be neglected, if the incoming particle is very much smaller compared to target particle (Tannouji 1977).

4. Result and Discussion

Total electron scattering cross section is obtained, as follows

$$\sigma = \frac{64\pi m D_e^{\,2} a^2 e^{2\alpha}}{\hbar^2}\frac{1}{E}\left(\begin{array}{l} e^{2\alpha}\dfrac{1}{6}\left(\dfrac{1}{64a^6} - \dfrac{\hbar^6}{\left(4a^2\hbar^2+8mE\right)^3}\right) \\ -2e^{\alpha}\dfrac{1}{27a^4}\left\{\begin{array}{l}\dfrac{1}{a^2}\ln\left(\dfrac{a^2\hbar^2+2mE}{a^2\hbar^2+8mE}\right) \\ -\dfrac{6}{16}\dfrac{\hbar^2}{\left(a^2\hbar^2+2mE\right)} - \dfrac{6}{4}\dfrac{\hbar^2}{\left(a^2\hbar^2+8mE\right)} + \dfrac{7}{8a^2}\end{array}\right\} \\ +\dfrac{1}{6}\left(\dfrac{1}{a^6} - \dfrac{\hbar^6}{\left(a^2\hbar^2+8mE\right)^3}\right)\end{array}\right) \tag{5}$$

From the result of calculation, model for electron scattering by diatomic hydrogen molecule is made, with dissociation energy 4.7446 eV, electron mass 9.11×10^{-31} kg, Morse parameter for hydrogen α 1.440558, and the distance between constituting atoms of the hydrogen molecule r_e 0.7416 Å, electron charge 1.6022×10^{-19} C, reduced Planck constant 1.054×10^{-34} Js. The graph of calculation result and experimental data is then compared.

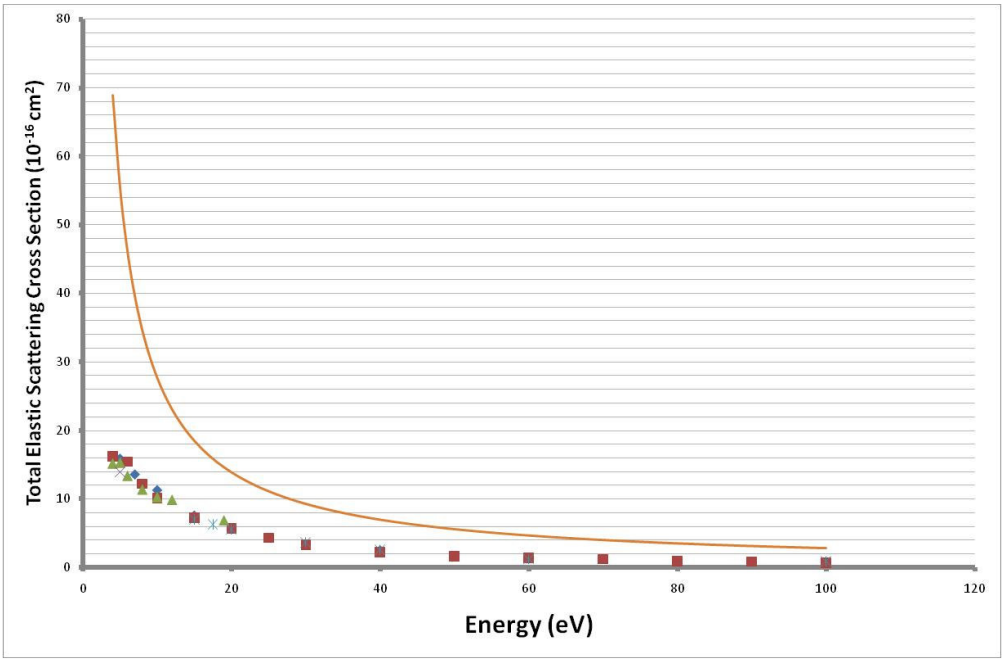

Figure 1. Comparison between calculated electron cross section by diatomic hydrogen molecule with secondary data from Brunger and Buckman (2002). The calculation result is shown by orange line, while experimental data is shown by dots.

In general, the graph of analytic calculation and experimental graph shows similar trend. Both graphs shows electron scattering cross section by diatomic molecule decreases as incoming electron energy increases, shows the decreasing of scattered electron probability by diatomic molecule as incoming electron energy increases.

The difference between experimental and theoretical values can be seen for energy range lower than 4.7 eV. For this energy range, the experimental cross section increases as electron energy increases, opposite with the general trend of the experimental cross section, and also theoretical result that shows cross section decreases as electron energy increases. For diatomic hydrogen, the dissociation energy is 4.7446 eV (Roy 2013). The incoming energy in this range is lower than the dissociation energy of the molecule. Incoming electron will be attracted by the nucleus of the molecule, which is positively charged, strong enough that it cannot escape from the molecule. Electrons experience recombination with the diatomic molecule. Therefore, fewer electrons are detected so that the value of experimental cross section decreases. Greater the energy of the incoming electron, greater the probability of escaping from the nuclear potential of the molecule, so the magnitude of total scattering cross section becomes greater as incoming electron energy increases.

For energy range between 4.7 eV to around 60 eV, the experiment result shows the cross section decreases as incoming electron energy increases. Theoretical approach shows the same trend, but the magnitude is bigger than the experimental value. In this range, electron has higher energy than dissociation energy of 4.7 eV, so that the electron can escape from nuclear potential, therefore there are more electrons detected by the sensor. The experimental value can be lower than the theoretical value might be due to breaking of incoming electron by electron cloud around the nucleus of diatomic molecule. In our theoretical model, the incoming electron is assumed to be free particle. Therefore, this can explain the difference in magnitude of experimental and theoretical value.

We compared the result of our calculation with the semi empirical formula by Liu and Sun (1996). Liu and Sun used double Yukawa potential and Additive Rule to find the total electron scattering cross section by diatomic molecules, via Born Approximation. Calculation result with Morse potential shows better trend with experimental value than double Yukawa potential. The model with Yukawa potential for electron-diatomic hydrogen intersects at around 20 eV energy. Although the value is small enough compared to the one with Morse potential at energy lower than 20 eV, the result for Yukawa model is higher than experimental value and does not show tendency to reach a common value for energy greater than 20 eV as shown in Figure 3. Thus, Morse potential better represents diatomic molecule than Yukawa potential.

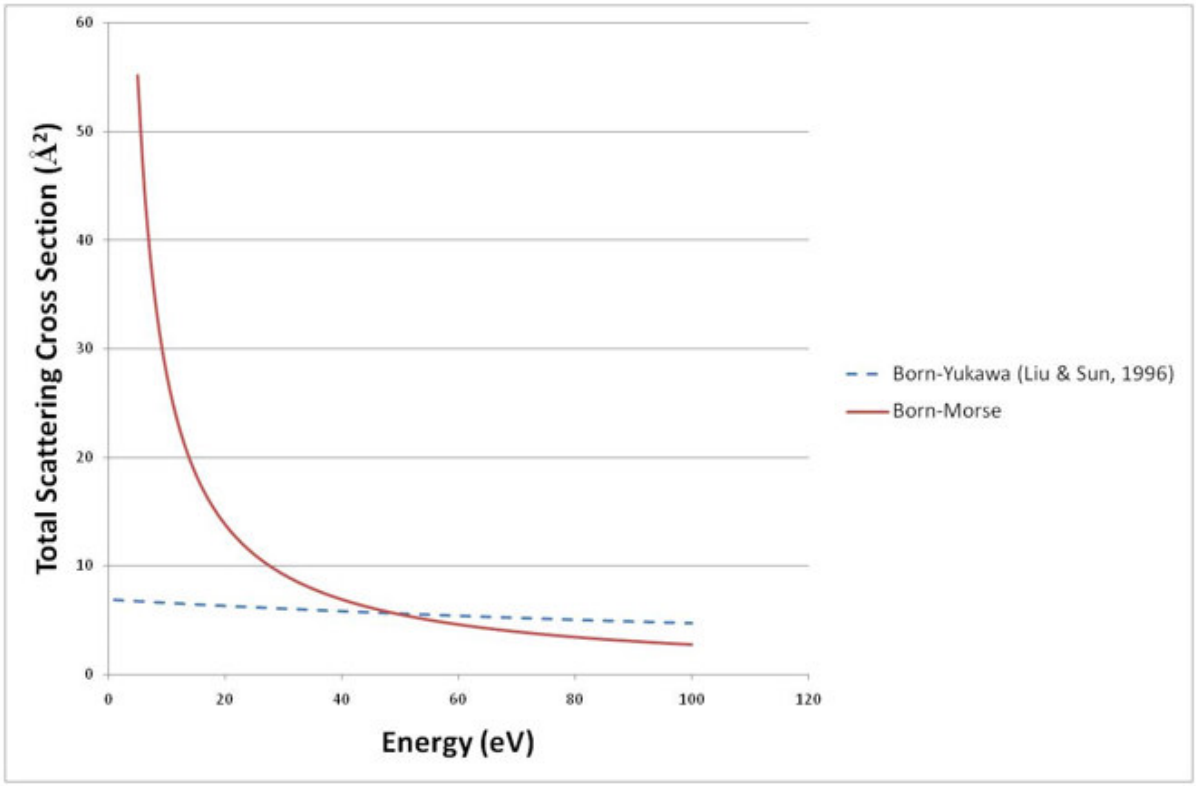

Figure 2. Comparison between theoretical calculation via Born Approximation and Morse potential and Born Approximation-double Yukawa potential derived by Liu and Sun for electron-hydrogen diatomic molecule.

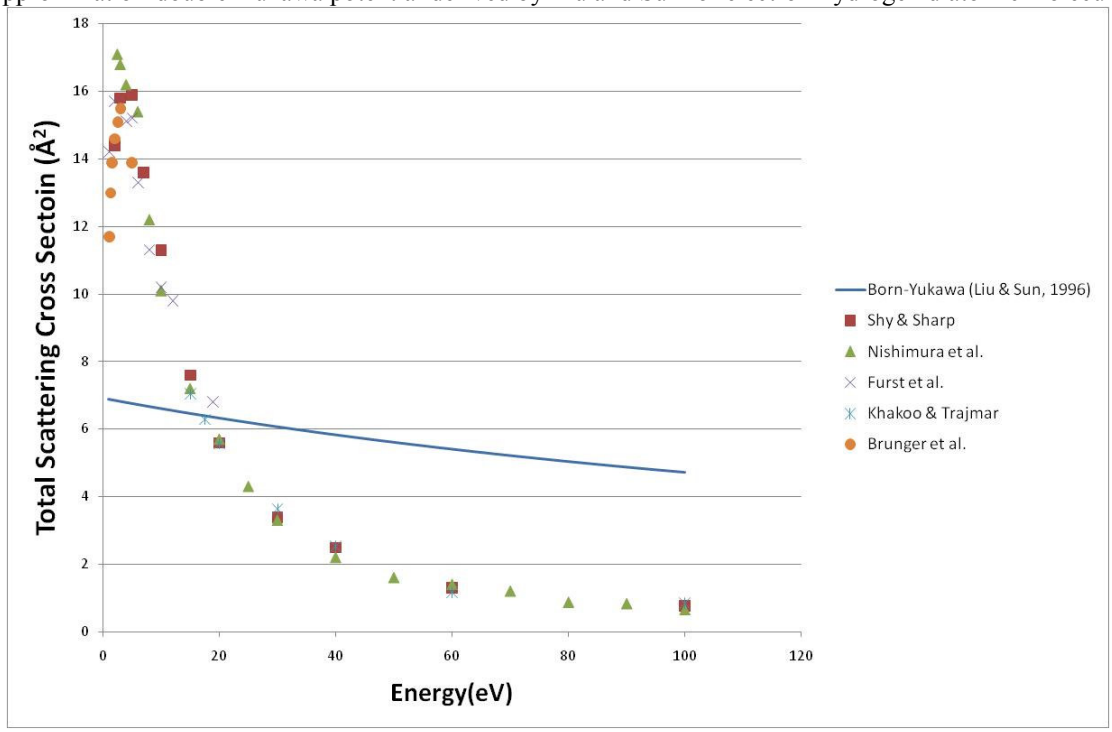

Figure 3. Comparison between semi empirical model from double Yukawa potential and experimental result for H2 molecule.

Model for electron scattering by O_2 is also made and compared with experimental data from Naghma et al.(2014), shown by Figure 4. Parameters used in this model are equilibrium distance between constituting atoms 1,207 Å Liu, Y. & Sun, J.(1996) and Naghma et al.(2014), and dissociation energy $8{,}19\times10^{-19}$ J Darwent, B. (1970). Model for O_2 gives similar trend with experimental result for energy higher than 100 eV. Morse parameter

α is obtained by fitting with experimental data. The value gives 1,4249 for O_2 molecules.

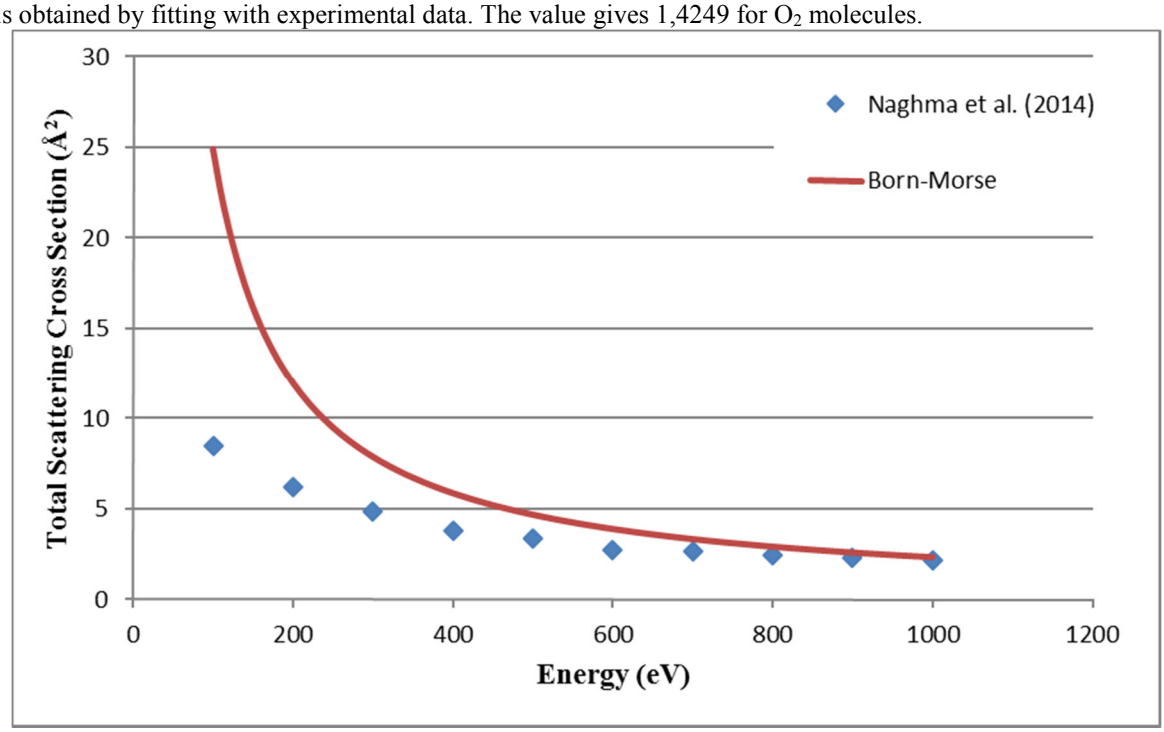

Figure 4. Comparison between calculation result with experimental data taken from Naghma et al. (2014) for O_2 molecule.

Electron scattering by S_2 is also made and compared with SCOP model by Naghma et al (2014), shown in Figure 5. The parameters used for S_2 are equilibrium distance between constituting atoms 1,889 Å Naghma et al (2014), and dissociation energy $7,13\times10^{-19}$ J Darwent, B. (1970). The model gives similar trend with SCOP model for S_2 for energy higher than 70 eV, although calculated values using Born approximation and Morse potential is higher than the ones in SCOP model. Morse parameter obtained from fitting gives the value of 1,446 for S_2 molecule.

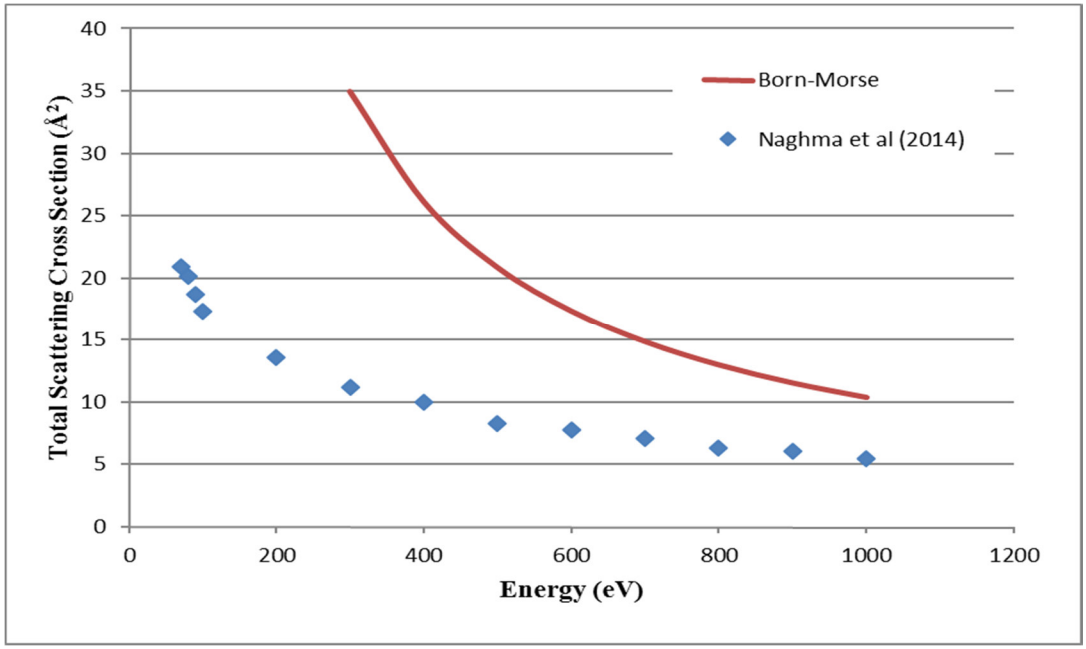

Figure 5. Comparison between calculation result and SCOP model by Naghma et al. (2014) for S_2 molecule.

5. Conclusion

Total electron scattering cross section by diatomic molecule is calculated using Born approximation and Morse potential. The value of electron scattering cross section decreases as incoming electron energy increases. The theoretical result for electron scattering by diatomic hydrogen molecule is modeled, and then compared with

experimental data. The theoretical value is higher than experimental value. Remembering the assumptions, the author mentioned earlier, and also the similarities between the trends of theoretical and experimental values for electron energy higher than 4.7 eV, we can conclude that Born approximation and Morse potential can be applied to calculate the total electron scattering cross section by diatomic molecules. We suggest that the same model be test to different type of diatomic molecules, either the ones that have identical atom such as O_2, N_2, etc. and also the ones with different constituting atoms such as CO, NO, etc. We also suggest adding approximation to correct inelastic scattering.

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