Total electron scattering cross sections of CH_4, C_2H_2, C_2H_4, and C_2H_6 in the energy range 200–1400 eV

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The total electron scattering cross section of CH_4, C_2H_2, C_2H_4, and C_2H_6 molecules have been obtained for 200–1400-eV energy electrons by measuring the attenuation of the electron beam through a gas cell. The present cross sections are compared to existing experimental cross sections as well as to theoretical predictions. The correlation between the total electron scattering cross section and the number of target-molecule electrons is discussed.

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I. INTRODUCTION

In recent years, there has been increased interest in the study of the total cross section for electron scattering from atoms and molecules at intermediate electron energies (400–5000 eV) [1–16]. Accurate cross-section measurements at these energies are required (1) to develop theoretical models in understanding the interaction process and (2) in applications in atmospheric physics, astrophysics, plasma physics, and chemical physics. In general, cross-section measurements above 400 eV energy are scarce, particularly for the simple hydrocarbons CH_4, C_2H_2, C_2H_4, and C_2H_6. Only three experimental groups have performed cross-section measurements of hydrocarbons above 400 eV energy; two of these are for CH_4 and the other is for C_2H_2. Zecca *et al.* [17] measured the total scattering cross section of CH_4 for 1–4000-eV energy electrons. Xing *et al.* [4] measured the cross sections of C_2H_2 for the energy range 400–2600 eV and made a comparison to the cross sections of CO, the isoelectronic partner of C_2H_2. Only one other measurement has been performed, recently by Garcia and Manero [3], for CH_4 for the energy range 400–5000 eV. Garcia and Manero found that their measurements are in agreement with the Bethe-Born theory [18] but 6–40% higher than those of Zecca *et al.* [17] for energies 1000 eV and above. No total electron scattering cross sections are reported in the literature for C_2H_4 and C_2H_6 above 400 eV energy.

The present experiment was undertaken to measure total electron scattering cross sections of CH_4, C_2H_2, C_2H_4, and C_2H_6 for 200–1400-eV electron energies. Although the cross sections of CH_4 and C_2H_2 have been measured previously [3,4,17] for this energy range, these measurements are repeated in this experiment for the comparison purposes. Further, the energy range was extended down to 200 eV to compare the cross-section measurements of C_2H_4 and C_2H_6 with those of Sueoka and Mori [19,20] in the energy range 1–400 eV. The present experimental cross sections are also compared with existing theoretical predictions. The correlation between the total electron scattering cross section and the number of target-molecule electrons is discussed.

II. EXPERIMENT

Given in Fig. 1 is the schematic of the experimental arrangement which was designed to measure the total electron scattering cross section based on the linear transmission technique. A Kimbal Physics Model EFG-7 electron gun was mounted on a vacuum chamber maintained in the low 10^{-7} Torr region. During the attenuation current measurement the pressure in the vacuum chamber was 1×10^{-5} Torr or better. A well-collimated narrow electron beam was obtained from the gun by passing the electron beam through three well-aligned 0.03 in. (0.76 mm) diameter apertures. Then the collimated electron beam, typically about 10^{-10}–10^{-13} A, enters the gas cell, which was defined by two apertures, 0.04 in. (1 mm) diameter, separated by 16–32 cm variable length. The gas pressure in the gas cell was measured by an MKS Baratron 126 A capacitance manometer. Electrons emerging from the gas cell enter a Comstock AC 902 double-focusing electrostatic analyzer (ESA) whose entrance is 4.5 cm away from the exit of the gas cell. The ESA was operated in 50 eV constant-energy transmission mode with 1 mm diameter entrance and exit apertures. At this setting the ESA energy resolution [full width at half maximum (FWHM)] is 0.75 eV or better. The ESA has been used in the past in collecting Auger spectra in eight different experiments [21] where the transmission properties, resolution, energy scale, and efficiency have been discussed. The ESA energy scale, measured to 0.1 eV or better, has been calibrated against the argon LMM and neon KLL Auger lines. In the present experiment transmitted electrons were collected on a Faraday cup and the intensity was measured

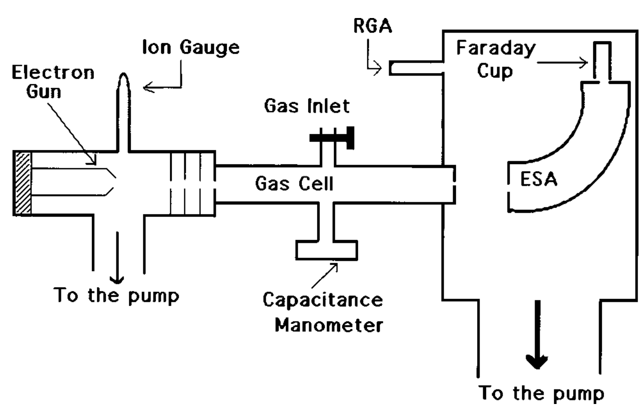

FIG. 1. The experimental arrangement.

by a Keithley Model 6517-A electrometer. Both ESA and Faraday cup were housed in a vacuum chamber maintained at 1×10^{-6} Torr or better. During the beam intensity measurement with gas present in the gas cell the pressure in this region was maintained at 1×10^{-5} Torr or better. The ESA, gas cell, electron gun, and entire electron optics system were shielded from the earth's magnetic field and other stray magnetic fields by 0.06 in. thick μ metal.

III. PROCEDURE AND ERRORS

The experimental procedure is based on the measurement of electron beam intensity attenuation through a gas. The intensities of the primary beam and attenuated beam, respectively, are I_0 and I,

$$I=I_0e^{-\sigma npL},$$

where n is the number density of molecules at 1 mTorr pressure, p is the pressure in units of mTorr, L is the electron-gas interacting length in m, and σ is the total electron scattering cross section in m^2. According to this relationship the variation of $\ln(I/I_0)$ with the pressure (p) in mTorr is a straight line whose slope is a measure of the total scattering cross section. An accurate determination of scattering cross section requires an accurate measurement of p, I_0, I, and L.

In the present experiment, the pressure was measured by an MKS Baratron 626 A capacitance manometer. Possible errors in the pressure measurement by this device are mainly due to the zero drifts in the scale and the temperature differences between the capacitance manometer head and the gas chamber. According to the manufacturer's specifications, the combined error due to zero drifts and temperature differences is estimated to be 2% or less.

The primary beam current (I_0) and attenuated beam current (I) were measured using the ESA, Faraday cup, and electrometer combination. Since the ESA deflects inelastically scattered forward electrons, I_0 and I could be measured accurately by passing the electron beam through the gas cell and measuring the current on the Faraday cup in the absence and in the presence of the gas. However, in this method electrons elastically scattered in the forward direction are not distinguished. In the present experiment the solid angle subtended by the entrance of the ESA and center of the gas cell is about 1.2×10^{-5} sr. Contributions from the 0° elastic scattering to this solid angle were estimated by extrapolating the experimental elastic scattering differential cross sections determined by Fink, Jost, and Herrmann [22] for C_2H_2, C_2H_4, and C_2H_6. It was found that the greatest error due to the contribution of 0° elastic scattering is about 0.5% for the energies and gases in the present experiment.

The gas-electron interaction length (L) is the only other measurement required to determine the total scattering cross section in this experiment. Considering the effect of effusion, the interaction length can be written as [4] $L=L_g+d_1+d_2+L_p$, where L_g is the geometric length, d_1 and d_2 are the diameters of the apertures of the gas cell, and L_p is the correction factor due to the differential pumping conditions. In the present experiment L_g is 24.5 cm, d_1 and d_2 are about 1 mm each, and L_p is estimated [23] to be about 2 mm. Therefore the interaction length in this experiment is essentially the geometrical length with 2% or less error. Also, several authors [3,4,17] have shown that the effective length is essentially the geometrical length if the geometrical length is 15 cm or greater. In order to verify this statement for the present experimental setup, the total scattering cross section of N_2 was measured for 400–1200-eV electron energies for three different gas-cell lengths, 16.0, 24.5, and 32.0 cm. These cross sections were found to be independent of the gas-cell length within the experimental uncertainties and agree well with those published in the literature [24]. A gas-cell length of 24.5 cm was used in the measurements of the listed cross sections in this paper.

The cross sections in the present experiment were performed using 10^{-10}–10^{-13} A electron currents and 0.5–10 mTorr gas pressures. For these current and pressure ranges no dependence of the cross section was found either on current or on pressure. In order to avoid possible systematic errors due to the small drift in electron current, the following procedure was adopted during the data collection. First, the electron beam was passed through the gas cell in the absence of the gas, and the current reading (I_0) on the Faraday cup was recorded. Then the gas cell was filled with the gas to a preselected pressure and the attenuated current (I) was recorded. Thereafter the gas inlet was closed and the gas cell was pumped down to 10^{-6} Torr or lower pressure and the beam current was monitored to make sure the nonattenuated current returns to its initial value (I_0). This procedure was followed for every set of I_0 and I measurements. The error due to the drift in current during the experiment is 0.5% or less for 200–1300 eV energies and 2–3 % for 1400 eV energy.

Research-grade target gases of CH_4, C_2H_2, C_2H_4, and C_2H_6 from Mattheson Co., Laporte, Texas, all within minimum purity 99.5% or better, were used. An on-site RGA, attached to the vacuum system where the ESA was housed, was used to make sure there was no air leak or other gas contaminant in the gas transport system.

Errors in the electron scattering cross-section measurements are as follows: (1) determination of interaction length (2%); (2) pressure measurement (2%); (3) contribution of 0° elastic scattering (0.5%); (4) beam current measurement, including the possible drift in the current during the experiment (1%); (5) statistical errors in determination of the slope (1%). These random errors combine in quadrature to give an overall error assignment of 3% or less for the electron energies 200–1300 eV. At 1400 eV the beam current was not as stable as at other energies. As a result there is an additional 3% error, giving a total error of 5% or less, in the measurements at this energy.

IV. RESULTS

The variation of $\ln(I/I_0)$ with the pressure of C_2H_6 gas is given in Fig. 2 for several electron energies between 200 and 1400 eV. The variation of $\ln(I/I_0)$ with pressure for the gases CH_4, C_2H_2, and C_2H_4 also demonstrated the same type of pattern. The experimental points lie on a straight line whose

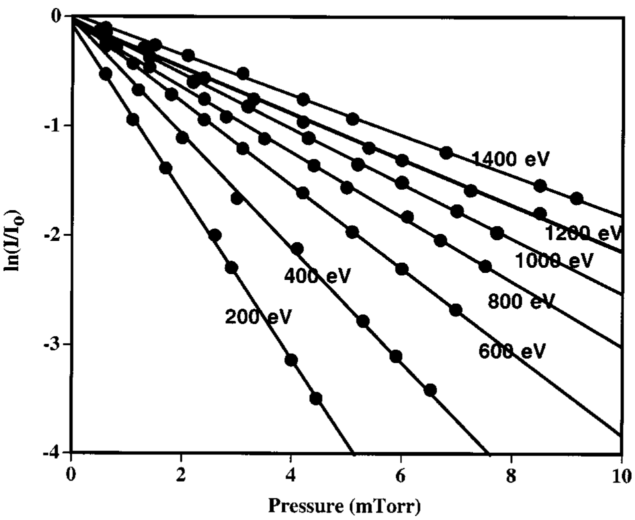

FIG. 2. Variation of $\ln(I/I_0)$ with pressure for C_2H_6 gas at selected energies ranging from 200 to 1400 eV.

slope is equivalent to the product of the number density per mTorr (n), the gas-electron interaction length (L), and the total scattering cross section (σ). Using the number density 3.5×10^{19} m^{-3} per mTorr and the interaction length 24.5 cm, these slopes were converted into cross sections. For a given electron energy, cross sections obtained in this manner for four to five independent experimental runs were averaged. Listed in Table I are the averaged cross sections as a function of energy.

V. DISCUSSION

There are three primary theoretical approaches to predicting the total electron scattering cross sections: (1) the Bethe-Born approximation [25,26], (2) the spherical complex optical potential (SCOP) method [14], and (3) the additivity rule method [27]. The Bethe theory defines the total inelastic cross section while the Born approximation gives the total elastic cross section. Therefore the combined Bethe-Born theory [25] expresses the total cross section (σ) in terms of the following analytical formula:

$$\frac{E}{R}\,\frac{\sigma}{\pi a_0^2}=A_{\rm el}+B_{\rm el}\frac{R}{E}+C_{\rm el}\left[\frac{R}{E}\right]^2+4M_{\rm tot}^2\ln\left[4c_{\rm tot}\frac{E}{R}\right],$$

where E is the incident energy in eV, R is the Rydberg energy, a_0 is the Bohr radius, and $A_{\rm el}$, $B_{\rm el}$, $C_{\rm el}$, $M_{\rm tot}$, and $C_{\rm tot}$ are constants that depend on the physical properties of the target molecule. These constants have been calculated [14] for several molecules, including CH_4 and C_2H_2, but not for C_2H_4 and C_2H_6.

In the SCOP method, a complex optical potential is constructed based on molecular wave functions and charge densities and is employed to determine the total cross sections. Several authors [10,13,14,27] have employed this method and calculated the cross sections for many molecules, including CH_4, C_2H_2, and C_2H_4.

The additivity rule, first introduced by Joshupura and Vinodkumar [27], predicts the total cross section (σ) as

$$\frac{\sigma}{a_0^2}=A\left[\frac{E_0}{\rm keV}\right]^{-B},$$

where E_0 is the electron energy in keV, A and B are parameters that depend on the molecular properties of the target gas, and a_0 is the Bohr radius. Based on this equation, Garcia and Monero [12] proposed an empirical model for the cross sections at intermediate electron energies (500–5000 eV). In this model,

$$\frac{\sigma}{a_0^2}=\left(0.4Z+0.1\frac{\alpha}{a_0^2}+0.7\right)\left(\frac{E}{\rm keV}\right)^{-0.78},$$

where Z and α are, respectively, the number of electrons in the target molecule and the polarizability (in units of a_0) of the target molecule.

Figures 3–6 display the variation of experimental cross sections produced in the present experiment with the electron energy. In the same figures the experimental cross sections produced in other laboratories as well as the existing theoretical predictions are given for comparison. As can be seen from Fig. 3, the experimental cross sections produced in the present experiment are in good agreement with those of others within the experimental uncertainties, except at 200 eV energy. At this energy the cross-section measurements in the present experiment are in agreement with the measurement of Sueoka and Mori [19] but about 7–8 % less than the one by Dababneh *et al.* [28]. The cross sections predicted by the model proposed by Garcia and Manero [12] are in very good agreement with the experimental values, but the predictions by Jain and Baluja (Bethe-Born approximation) [14] are consistently lower (5–12 %) than the experimental values. The theoretical predictions by Jiang, Sun, and Wan [13], available only up to 1000 eV energy, do not follow the same variation as the experimental cross sections. These cross sections are 5–15 % higher than the experimental values at energies be-

TABLE I. Total cross section for electron scattering on CH_4, C_2H_2, C_2H_4, and C_2H_6 in units of 10^{-20} m^2 for intermediate electron energies.

Energy (eV)	CH_4	C_2H_2	C_2H_4	C_2H_6
200	5.78 ± 0.20	6.52 ± 0.18	8.60 ± 0.22	8.83 ± 0.20
300	4.55 ± 0.18	5.48 ± 0.05	7.05 ± 0.20	7.51 ± 0.21
400	3.90 ± 0.07	5.12 ± 0.16	5.96 ± 0.16	6.42 ± 0.19
500	3.20 ± 0.13	4.50 ± 0.12	4.81 ± 0.16	5.31 ± 0.17
600	2.74 ± 0.06	3.99 ± 0.11	4.06 ± 0.14	4.60 ± 0.13
700	2.44 ± 0.10	3.53 ± 0.13	3.73 ± 0.11	4.11 ± 0.15
800	2.19 ± 0.06	3.10 ± 0.11	3.43 ± 0.07	3.63 ± 0.15
900	2.08 ± 0.05	2.88 ± 0.11	3.13 ± 0.09	3.40 ± 0.14
1000	1.83 ± 0.07	2.62 ± 0.09	2.93 ± 0.12	3.06 ± 0.12
1100	1.71 ± 0.07	2.42 ± 0.10	2.67 ± 0.10	2.82 ± 0.13
1200	1.57 ± 0.05	2.23 ± 0.08	2.40 ± 0.09	2.55 ± 0.11
1300	1.46 ± 0.07	1.95 ± 0.08	2.15 ± 0.10	2.30 ± 0.09
1400	1.36 ± 0.10	1.85 ± 0.09	1.94 ± 0.12	2.15 ± 0.12

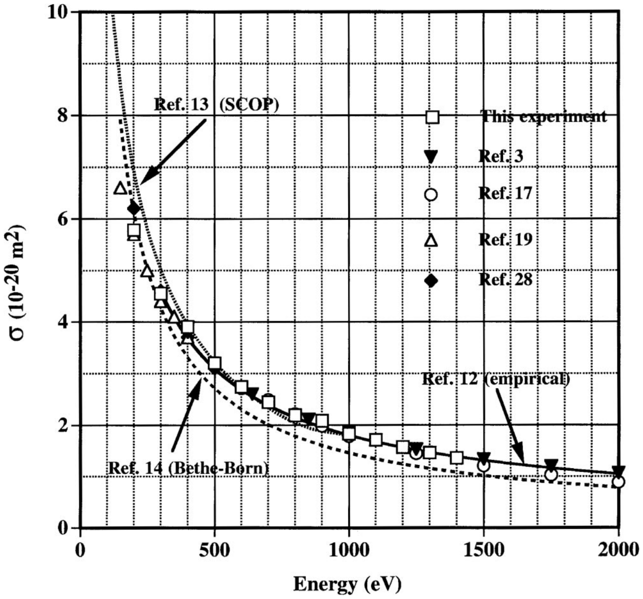

FIG. 3. Total electron scattering cross sections of CH_4 in 10^{-20} m^2. Open squares are the present measurements. Solid inverted triangles, open circles, open triangles, and solid diamonds are, respectively, the experimental cross sections of Garcia and Manero [3], Zecca *et al.* [17], Sueoka and Mori [19], and Dababneh *et al.* [28]. The dotted, dashed, and solid lines are, respectively, the theoretical predictions by Jing, Sun, and Wan [13], Jain and Baluja [14], and Garcia and Manero [12].

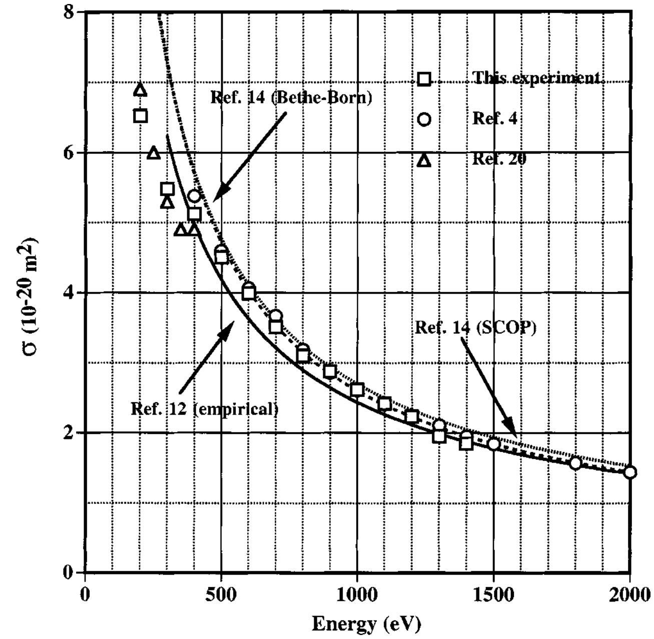

FIG. 4. Total electron scattering cross sections of C_2H_2 in 10^{-20} m^2. Open squares are the present measurements. Open circles are by Xing *et al.* [4] and open triangles are by Sueoka and Mori [20]. The dotted and dashed lines are, respectively, the theoretical predictions by the SCOP method (Jain and Baluja [14]) and by Bethe-Born theory (Jain and Baluja [14]) while the solid line is the theoretical prediction by an empirical model of Garcia and Manero [12].

low 500 eV while in the energy range 600–1000 eV there is near agreement between theoretical predictions and experimental values.

As can be seen from Fig. 4 the experimental cross sections of C_2H_2 produced in this investigation are in good agreement with those of Xing *et al.* [4] for the energy range 400–1400 eV. Also, the cross sections produced in this laboratory below 400 eV energy are in fair agreement with those of Sueoka and Mori [20]. For C_2H_2, both the theoretical predictions by Jain and Baluja [14] (one based on the Bethe-Born approximation and the other based on the spherical complex optical potential method) are in close agreement with the experimental values for energies higher than 500 eV. But for energies lower than 500 eV, the predictions by both models are 10–20 % higher than the experimental cross sections. Also, the predictions based on the model proposed by Garcia and Manero [12] are 2–10 % lower than the experimental values for energies 500 eV and above where the model is applicable.

As displayed in Fig. 5, the experimental cross sections of C_2H_4 produced in this experiment in the 200–400 eV energy range are 7–10 % higher than those of Sueoka and Mori [19]. No other experimental cross sections are available for comparison with the present measurements to our knowledge. It is interesting to see that the theoretical predictions by the model proposed by Garcia and Manero [12] are in very good agreement with the experimental values for the entire energy range in this experiment. But the theoretical predictions by Jian, Sun, and Wang [13] are 0–30 % higher than the experimental values, with the greatest deviation at lower

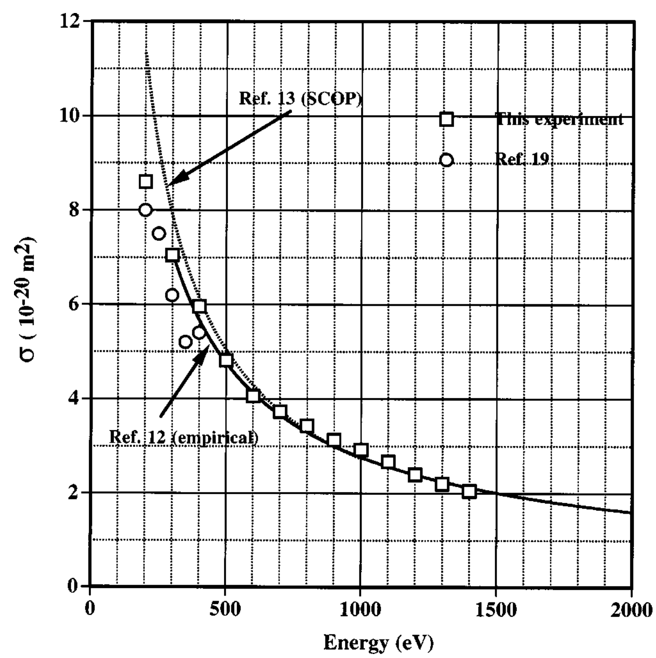

FIG. 5. Total electron scattering cross sections of C_2H_4 in 10^{-20} m^2. Open squares are the present measurements while the open circles are the measurements by Sueoka and Mori [19]. The solid curve is the prediction by Garcia and Manero [12] while the dotted curve is the theoretical prediction by Jian, Sun, and Wan [13].

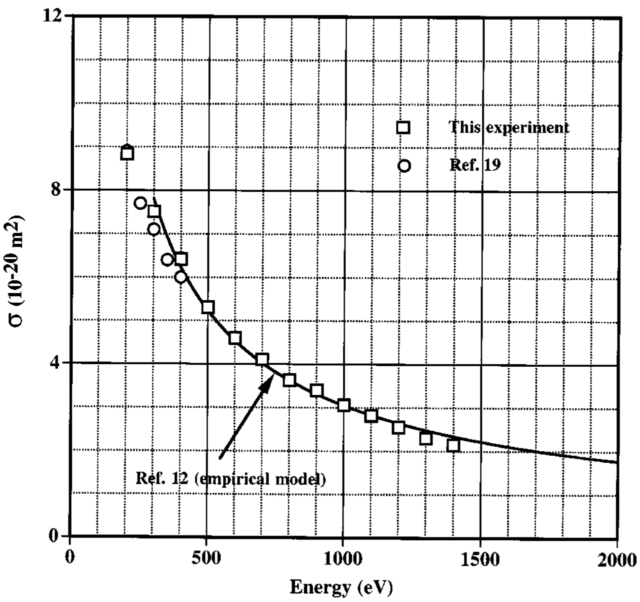

FIG. 6. Total electron scattering cross sections of C_2H_6 in 10^{-20} m^2. Open squares are the present measurements while the open circles are the measurements by Sueoka and Mori [19]. The solid curve is the prediction by Garcia and Manero [12].

energies. In Fig. 6, where the experimental cross sections of C_2H_6 produced in the present experiment are compared with those of the model proposed by Garcia and Manero [12], it is clear that the model agrees closely with the experimental measurements. No theoretical cross sections based on the Bethe-Born approximation or the SCOP method are available for comparison. As can be seen from Fig. 6, the experimental values of Sueoka and Mori [19] for C_2H_6 are in close agreement with those of the present experiment in the region where the energies of the two experiments overlap.

Both experimentalists [4,11,12,29] and theorists [14] have discussed the correlation between the number of target-molecule electrons and the total electron scattering cross section. In order to examine this feature further, the experimental cross sections produced in this experiment were scaled as a function of the number of target electrons in the molecule for 200–1400 eV projectile electron energies (Fig. 7). In the same figure the experimental cross sections at lower energies

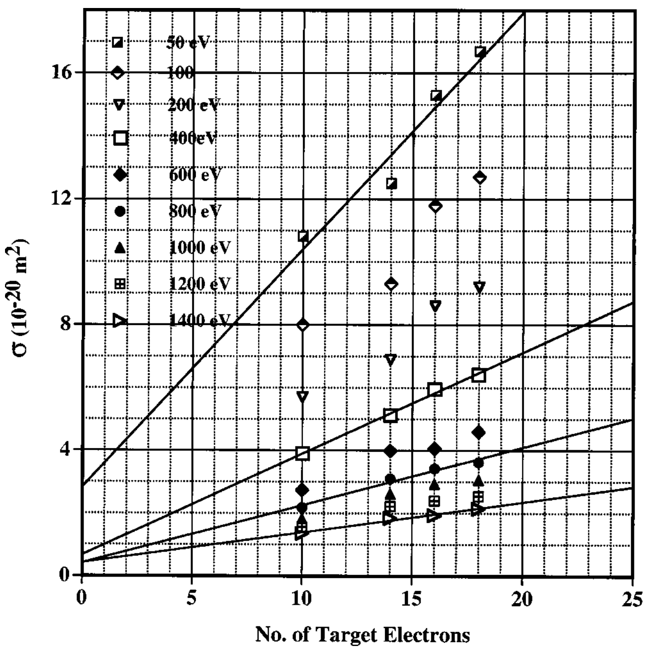

FIG. 7. Variation of the total cross section with the number of target electrons for selected energies between 50 and 1400 eV.

(50 and 100 eV) of Sueoka and Mori [19,20] are scaled accordingly. This figure clearly shows a linear relationship between the measured total electron scattering cross section and the number of electrons in the target molecule. Currently another experiment is in progress to study this correlation further.

VI. CONCLUSION

Total electron scattering cross sections of CH_4, C_2H_2, C_2H_4, and C_2H_6 have been measured for 200–1400-eV electrons. The measured cross sections are in good agreement with the empirical model proposed by Garcia and Mori [12] for CH_4, C_2H_4, and C_2H_6, but the model underpredict the cross sections of C_2H_2. A nearly linear relationship is evident between the total scattering cross section and the number of target-molecule electrons for the energy range 50–1400 eV for the four molecules CH_4, C_2H_2, C_2H_4, and C_2H_6.

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