Absolute elastic differential electron scattering cross sections in the intermediate energy region. IV. CO[a)]

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(Received 18 August 1978)

Using a crossed electron beam–molecular beam scattering geometry and a relative-flow technique, ratios of elastic differential cross sections of CO to those of He have been measured at electron impact energies of 3, 5, 7.5, 9.9, 15, 20, 30, 50, 75, and 100 eV. At each energy, an angular range of 15° to 130° has been covered. These ratios have been multiplied by previously known He elastic differential cross sections to obtain elastic differential cross sections for CO. Since pure rotational excitations were not resolved, the elastic differential cross sections are a sum of elastic and pure rotational excitations at room temperature. From a knowledge of differential cross sections (DCS), integral and momentum transfer cross sections have been calculated. Both the DCS and integral cross sections are compared at 50, 75, and 100 eV to a recent two-potential theory of e–molecule scattering. Present results show that the isoelectronic molecules CO and N_2 have very similar magnitudes and shapes of their differential cross sections.

I. INTRODUCTION

Properties of the CO molecule have become increasingly important in recent years because of its laser action in the high-pressure pulsed-discharge system,[1] public concern over the consequences of air pollution, and its presence in diffuse interstellar clouds.[2,3] Even more recent is its importance in the understanding and modeling of the atmospheric convection on Jupiter.[4]

From the theoretical point of view, the present elastic differential cross sections (DCS) are capable of providing important tests of e–molecule scattering theories. Moreover, the fact that CO and N_2 are ioselectronic should provide interesting intercomparisons of the two sets of DCS's. For example, DCS's for the two gases have been found to be very similar to one another at high electron energies where data[5,6] on both are available.

Quantitative electron-impact cross section measurements on CO are less extensive and less precise than the studies of its negative ion resonances.[7-9] The angular distribution of elastically scattered intensity of electrons was measured by Ramsauer and Kollath[10] in the 0.99–6.25 eV region for the angular range 15°–167.5°, and by Arnot[11] in the 30–785 eV region for the angular range 10°–120°. At relatively high electron energies, Bromberg[5,6] made absolute measurements in the 205–500 eV region for the angular range 3°–35°. More recently, absolute differential elastic cross sections were obtained by DuBois and Rudd[12] in the 200–800 eV region for the angular range 2°–150°. At intermediate energies, the only experimental results are normalized absolute cross sections[13] at 20 eV and relative measurements over the angular range 15°–85° at other energies.[14]

In the present paper, we report the first absolute values of DCS for CO at impact energies of 3–100 eV for the angular range 15°–135° as part of a current program in this laboratory to determine absolute DCS of gases of interest in lasers, plasmas, and in the Earth's and other planetary atmospheres. Also reported are corresponding integral and momentum-transfer cross sections. In Sec. II, we briefly describe the methods employed in these measurements. In Sec. III, our experimental results are presented and compared with previous CO measurements, the DCS of N_2,[15] and a two-potential theory of e–molecule scattering at intermediate and high energies.[16]

II. APPARATUS AND METHOD

The apparatus used in the measurements have been described previously.[17,18] It consists of a crossed target–electron beam geometry. The target molecular beam is produced by flowing CO through a capillary array. The mechanical arrangement consists of a fixed array and electron energy analyzer, and an electron gun which is rotatable about the scattering volume over the angular range $-30°$ to $+135°$. The electron optics are energy compensated in the sense that its focusing properties are independent of the final electron energy.[18] Incident currents are 2–8 nA at a resolution of about 65 meV (FWHM), and the solid angle of detection about 2×10^{-3} sterad.

The method[17] employs a measurement, at a constant electron impact energy, of the intensity of the elastically scattered electrons by the gas under experimental investigation (CO) to that of He. This ratio is related to the ratio of cross sections $\sigma(\mathrm{CO},\theta)/\sigma(\mathrm{He},\theta)$ according to

$$\sigma(\mathrm{CO},\theta)/\sigma(\mathrm{He},\theta)=[\dot{N}_e(\mathrm{CO})/\dot{N}_e(\mathrm{He})][m(\mathrm{He})/m(\mathrm{CO})]^{1/2}\times[\dot{N}_b(\mathrm{He})/\dot{N}_b(\mathrm{CO})]\,, \quad (1)$$

$$=[\dot{N}_e(\mathrm{CO})/\dot{N}_e(\mathrm{He})][p(\mathrm{He})/p(\mathrm{CO})]\,, \quad (2)$$

where $\dot{N}_e(\mathrm{CO})$ and $\dot{N}_e(\mathrm{He})$ are the experimentally measured intensities (as integrated peak counts) of elastically scattered electrons, $m(\mathrm{He})$ and $m(\mathrm{CO})$ are molecular weights, $\dot{N}_b(\mathrm{He})$ and $\dot{N}_b(\mathrm{CO})$ are flow rates of the

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TABLE I. CO differential elastic cross sections $\sigma(\mathrm{CO}, \theta)$ in units of 10^{-20} $\mathrm{m^2/sterad}$. In parentheses are the ratios $\sigma(\mathrm{CO}, \theta)/\sigma(\mathrm{He}, \theta)$.

E_0 (eV) / θ (deg)	3	5	7.5	9.9	15	20	30	50	75	100
15	2.17	1.61	1.95	2.13	3.90	5.12	3.78	3.77	3.82	2.89
	(9.87)	(6.13)	(4.79)	(5.19)	(7.59)	(8.91)	(6.07)	(6.29)	(7.85)	(7.32)
20	2.76	1.97	1.77	2.10	3.29	4.01	2.96	2.54	2.38	1.86
	(12.0)	(7.52)	(5.51)	(5.43)	(7.02)	(7.84)	(5.49)	(5.31)	(6.49)	(6.40)
30	2.81	2.10	1.67	1.83	2.41	2.24	1.72	1.20	0.879	0.592
	(11.1)	(7.85)	(5.50)	(5.34)	(6.11)	(5.53)	(4.29)	(3.87)	(4.11)	(3.66)
40	3.21	2.27	1.62	1.83	1.44	1.47	0.886	0.507	0.328	0.222
	(11.4)	(8.15)	(5.54)	(5.84)	(4.29)	(4.55)	(2.98)	(2.46)	(2.49)	(2.32)
50	3.14	1.98	1.41	1.41	1.10	0.679	0.474	0.243	0.147	0.134
	(10.0)	(6.66)	(4.85)	(4.77)	(3.77)	(2.56)	(2.11)	(1.68)	(1.69)	(2.17)
60	2.49	1.65	1.11	1.02	0.74	0.477	0.262	0.138	0.0947	0.0910
	(7.08)	(5.08)	(3.70)	(3.57)	(2.83)	(2.11)	(1.48)	(1.30)	(1.53)	(2.13)
70	1.87	1.40	0.82	0.67	0.48	0.301	0.183	0.0884	0.0696	0.0771
	(4.79)	(3.93)	(2.61)	(2.32)	(1.95)	(1.49)	(1.25)	(1.07)	(1.50)	(2.48)
80	1.22	1.06	0.62	0.51	0.32	0.203	0.122	0.0650	0.0671	0.0632
	(2.82)	(2.69)	(1.83)	(1.71)	(1.33)	(1.08)	(0.96)	(0.97)	(1.86)	(2.70)
90	0.96	0.84	0.48	0.39	0.32	0.226	0.110	0.0625	0.0626	0.0571
	(2.01)	(1.94)	(1.29)	(1.21)	(1.31)	(1.24)	(0.96)	(1.10)	(2.15)	(3.14)
100	0.69	0.70	0.41	0.48	0.36	0.256	0.121	0.0740	0.0725	0.0582
	(1.31)	(1.47)	(1.03)	(1.39)	(1.41)	(1.41)	(1.13)	(1.48)	(2.96)	(3.93)
110	0.52	0.65	0.49	0.55	0.46	0.306	0.148	0.106	0.0745	0.0560
	(0.91)	(1.25)	(1.12)	(1.49)	(1.73)	(1.66)	(1.44)	(2.33)	(3.45)	(4.41)
120	0.52	0.72	0.60	0.69	0.58	0.392	0.219	0.146	0.0995	0.0627
	(0.86)	(1.28)	(1.25)	(1.74)	(2.06)	(2.05)	(2.13)	(3.43)	(5.00)	(5.45)
130	0.59	0.81	0.73	0.79	0.69	0.496	0.318	0.213	0.125	0.0701
	(0.91)	(1.35)	(1.42)	(1.85)	(2.33)	(2.47)	(3.01)	(5.20)	(6.54)	(6.61)
σ_I (10^{-20} $\mathrm{m^2}$)	18	15	11	12	11	9.9	6.6	5.5	4.0	3.0
σ_M (10^{-20} $\mathrm{m^2}$)	13	12	9.7	10	8.5	6.7	4.1	3.2	1.6	1.1

two gases into the scattering chamber as measured by flow meters, and p(He) and p(CO) are pressures behind the capillary array. These quantities and derivations are described in detail in Ref. 17. By this method, we obtain the ratio of differential cross sections. The absolute value $\sigma(\mathrm{CO}, \theta)$ is calculated by multiplying this ratio by the absolute value of $\sigma(\mathrm{He}, \theta)$. Thus, the cross sections $\sigma(\mathrm{He}, \theta)$ are used as secondary standards.

As in all previous studies, certain precautions were taken to minimize sources of errors. They have been discussed in detail in Ref. 17.

III. RESULTS AND DISCUSSION

Using the relative-flow technique described above, ratios were obtained of the DCS of CO to those of He, at incident energies of 3, 5, 7.5, 9.9, 15, 20, 30, 50, 75, and 100 eV. The angular range covered was 15°–130° at each energy. As mentioned earlier, the energy resolution of the spectrometer was insufficient to resolve pure rotational transitions in CO. Since at about 250 K (corresponding to a slightly cooled beam effusing from the capillary array) the level of maximum population is $j=6$, the elastic DCS reported here are actually sums of elastic and rotational excitation cross sections involving j's as high as 15. The impact energy of 9.9 eV was chosen to avoid effects of the CO resonance at 10.04 eV.

Results of the present measurements are given in Table I. In parentheses are the DCS ratios of CO to those of He. Absolute values of the CO DCS are listed in Table I. These absolute values were obtained by multiplying the ratios by previously measured He cross sections. For the present work, at electron impact energies of 3, 5, 7.5, 9.9, and 15 eV, the He DCS data of Andrick and Bitsch[19] were used. Values of $\sigma(\mathrm{He}, \theta)$ at 7.5, 9.9, and 15 eV were obtained by interpolating their results at 7, 8, 10, 14, and 16 eV. At impact energies of 20, 30, 50, 75, and 100 eV, the DCS of He used were obtained in our laboratory.[20]

The estimated error in the measured ratios $\sigma(\mathrm{CO}, \theta)/\sigma(\mathrm{He}, \theta)$ is 10%. A summary of the possible sources of error are given in Table II of Ref. 17. Errors in the values $\sigma(\mathrm{CO}, \theta)$ are estimated to be 22% at 3 eV, 11% at 5–15 eV, and 15% at 20–100 eV. These errors are square roots of the quadratic sum of the 10% error in the ratio measurement and the error in $\sigma(\mathrm{He}, \theta)$. For this last error, Andrick and Bitsch[19] quote 20% at 3 eV,

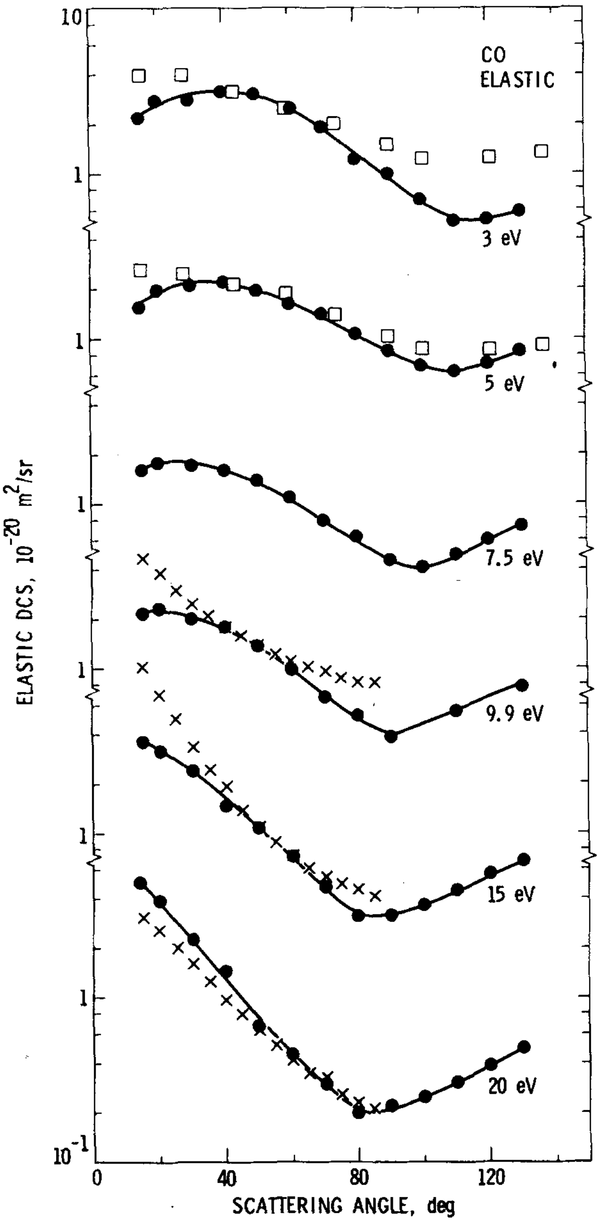

FIG. 1. Elastic DCS for CO between 3 and 20 eV. ●, present measurements joined by a smooth solid line; X, Truhlar *et al.*,[13,14] their data normalized to present results at $\theta = 50°$; □, Ramsauer and Kollath,[10] their 2.6 and 4.8 eV data compared with present results at 3 and 5 eV, respectively. Their relative results were normalized to the present data at $\theta = 43°$.

and 5% at 5–15 eV. At 20, 30, 50, 75, and 100 eV, our laboratory measurements are uncertain by about 15%.

Figures 1 and 2 show the present results of $\sigma(\mathrm{CO}, \theta)$ as a function of θ at energies of 3–100 eV. These results are compared with experimental values of Ramsauer and Kollath,[10] Arnot,[11] and Truhlar *et al.*[13,14] Since these various measurements were in arbitrary units, they were, for the purpose of presentation in Figs. 1 and 2, placed on the absolute scale by normalization to the present measurements. Within limits of experimental error, the shapes of all normalized DCS are in satisfactory agreement with present measurements, except for the 3, 10, and 15 eV results. Low-angle discrepancies at 10 and 15 eV are due to volume-correction effects which may not have been taken into account very accurately in Ref. 14. The differences at 3 eV could arise from lingering effects of the CO shape resonance[7] at 1.7 eV, and the slightly different impact energy between present measurements and those of Ref. 10.

Also shown in Fig. 2 at 50, 75, and 100 eV are recent calculations of e–CO elastic scattering by Choi *et al.*[16] A two-potential approach is used in these calculations in which contributions to the scattering amplitude of a short-range potential (consisting of shielded nuclear Coulomb potential) and a long-range potential (consisting of multipole potentials of a permanent and induced nature) are added incoherently to give the final DCS. The absolute DCS calculated in this theory are seen to be about a factor of (at most) 3 higher than the present data. The agreement in *shape* of the measurements and calculations is very good.

Since N_2 is isoelectronic with CO, it may be reasonably expected to show some similarity in its DCS to that of CO. For example, the 1–0 pure vibrational cross sections in the two gases are generally similar in shape and magnitude.[21] Bromberg[5,6] found that CO and N_2

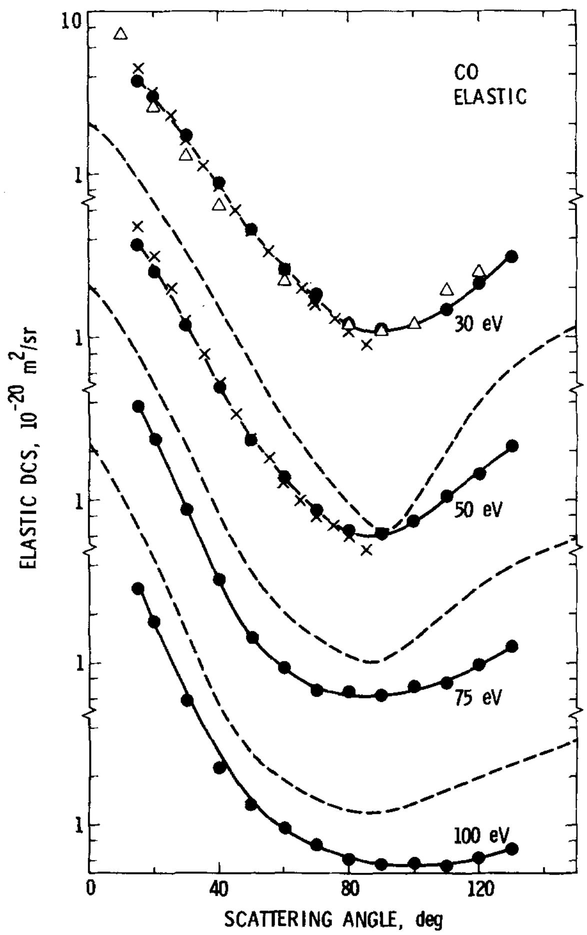

FIG. 2. Elastic DCS for CO between 30 and 100 eV. ●, present measurements joined by a smooth solid line; X, Truhlar *et al.*,[13,14] their data normalized to present results at $\theta = 50°$; Δ, Arnot,[11] data normalized to present measurements at $\theta = 50°$; ----, theoretical results of Choi *et al.*[16]

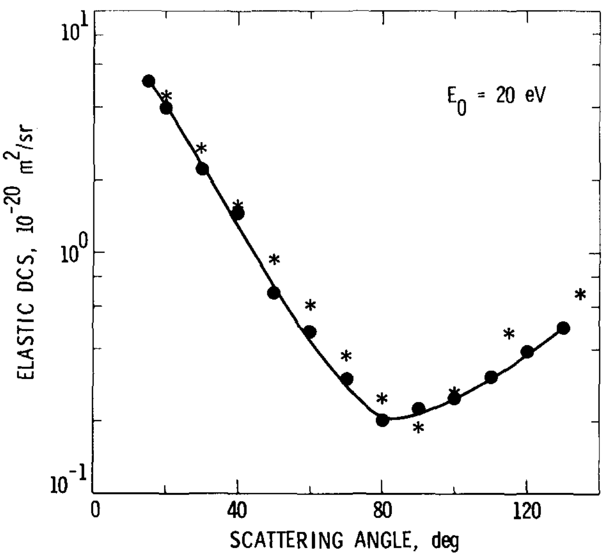

FIG. 3. Elastic DCS of CO and N_2 at 20 eV impact energy. DCS for CO have been joined by a smooth line giving a visual fit of the present data. ●, present measurements for CO; *, elastic DCS for N_2 of Srivastava *et al.*[15]

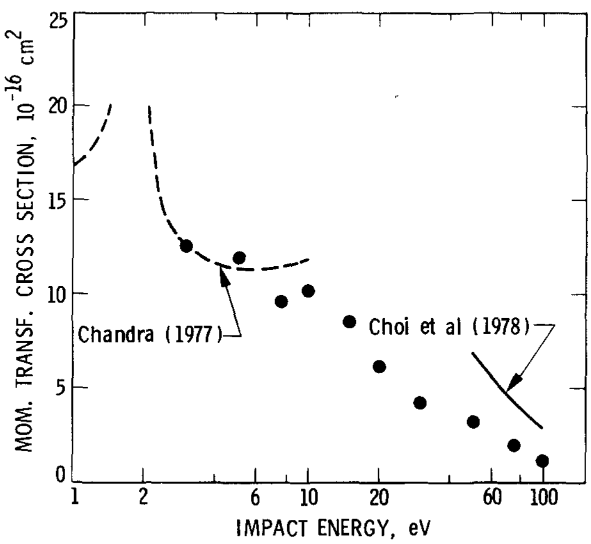

FIG. 5. Elastic momentum-transfer cross sections σ_M. ●, present measurements; ---, theoretical results of Chandra[25] for $j=0\rightarrow j=0$ elastic scattering only; —, theoretical results of Choi *et al.*[18]

have nearly the same elastic cross sections at energies of 300–500 eV. DuBois and Rudd[12] verified this at energies of 200, 500, and 800 eV. In the present work, it is found that, even at intermediate energies, CO and N_2 have similar DCS in both magnitude and shape over the measured angular range. A comparison at 20 eV of elastic DCS for N_2 as measured by Srivastava *et al.*[15] with that of CO is shown in Fig. 3. In general, it is

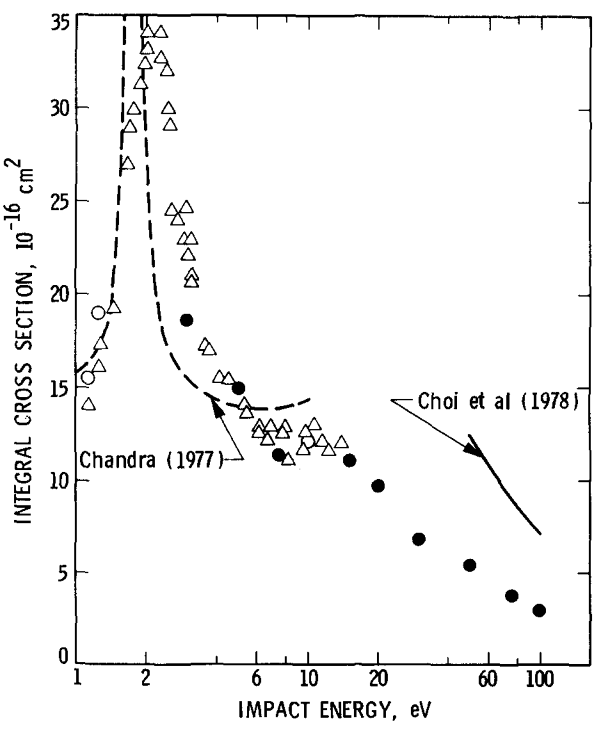

FIG. 4. Elastic integral cross sections σ_I. ●, present measurements; Δ, Brüche[23]; o, Ramsauer and Kollath[10]; ---, theoretical results of Chandra[25] for $j=0\rightarrow j=0$ elastic scattering only; —, theoretical results of Choi *et al.*[18]

found that these DCS at 5 eV are at most a factor of 1.5 lower than the CO data, while at other energies the N_2 DCS are at most a factor of 1.5 larger. One must therefore conclude that effects arising from small differences in the nuclear Coulomb potential of the two molecules, as well as effects of the long-range dipole potential in CO, must be small or cancel one another to some extent.

Also shown in Table I are integral (σ_I) and momentum-transfer (σ_M) cross sections calculated from, respectively,

$$\sigma_I = 2\pi \int_0^\pi \sigma(\mathrm{CO}, \theta) \sin\theta \, d\theta \tag{3}$$

and

$$\sigma_M = 2\pi \int_0^\pi \sigma(\mathrm{CO}, \theta) \sin\theta (1-\cos\theta) \, d\theta \,. \tag{4}$$

Since the range of θ covered in the data was $15° \leq \theta \leq 130°$, the DCS curves had to be extrapolated from 15°–0° and 130°–180°. For this purpose, two methods of extrapolation were used:

(1) 3–30 eV: There are no accurate theoretical calculations for e–CO elastic scattering in this energy range. Since empirically it was found that the N_2 and CO DCS were quite similar in shape, we decided to use the shape of Siegel *et al.*'s[22] recent theoretical N_2 cross sections to aid in the extrapolation of 0° and 180°. The main justification for this lies in the reasonable agreement (both magnitude and shape) between the two sets of experimental data.

(2) 50–75 eV: In this range, the shape of e–CO calculations of Choi *et al.*[16] were used in the low and high-angle extrapolations.

Estimated errors in σ_I at all energies are 20%, and those in σ_M are 30%. These errors are based on the error of the DCS itself, and on an estimate of the extrapolation errors to 0° and 180°.

Present integral cross sections may also be compared with earlier measurements of Brüche[23] and Ramsauer and Kollath,[24] and this comparison is shown in Fig. 4. The overall agreement is excellent, and it is interesting to note that the presence of a shoulder at an impact energy of 10 eV is confirmed in our data. We also show in Fig. 4 results of a recent calculation by Chandra[25] using a combined frame-transformation, R-matrix approach to the scattering problem. We have plotted in Fig. 4 his results for the $j=0 \rightarrow j=0$ transition only. Since the maximum population of CO at the temperature of the molecular beam is in $j=6$, one would have to sum the many elastic, inelastic, and superelastic contributions from j's as high as 15. Such theoretical results were not available, and we show in Fig. 4 only the elastic $j=0 \rightarrow j=0$ cross section. Corresponding theoretical and experimental values of the momentum-transfer cross section σ_M are presented in Fig. 5.

ACKNOWLEDGMENTS

We would like to thank Dr. J. Dehmer, Dr. D. Dill, and Professor R. T. Poe for supplying numerical results of their calculations. One of us (H. T.) would also like to thank Dr. S. Trajmar for his constant encouragement and guidance during the course of his NRC–NASA Resident Research Associateship.

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