

Absolute elastic differential electron scattering cross sections in the intermediate energy region. III. SF₆ and UF₆*†

Santosh K. Srivastava, S. Trajmar, A. Chutjian, and W. Williams

Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California 91103
(Received 14 November 1975)

A recently developed technique has been used to measure the ratios of elastic differential electron scattering cross sections (DCS) for SF₆ and UF₆ to those of He at electron impact energies of 5, 10, 15, 20, 30, 40, 50, 60, and 75 eV and at scattering angles of 20° to 135°. In order to obtain the absolute values of DCS from these ratios, He DCS of McConkey and Preston have been employed in the 20° to 90° range. At angles in the 90° to 135° range the recently determined cross sections of Srivastava and Trajmar have been utilized. From these DCS, elastic integral and momentum transfer cross sections have been obtained.

I. INTRODUCTION

A great need has developed recently in connection with various laser systems, the UF₆ gas core reactor, and isotope separation schemes for cross section data for electron-SF₆ and UF₆ collision processes. Theoretical methods are not expected to yield reliable cross sections for these large molecules. No experimental cross section data are available at the present time on UF₆ and only very limited data on SF₆. Some optical spectroscopical data are available but much more could be obtained concerning optically forbidden and far uv transitions by the methods of electron impact spectroscopy. Therefore, in this laboratory, we undertook a study of these gases. A first step in this direction was to measure absolute values of cross sections for the elastic scattering of electrons. They yield the elastic integral and momentum transfer cross sections, and make it possible to obtain absolute inelastic cross sections from conventionally measured inelastic to elastic scattering intensity ratios.

We present here absolute elastic scattering differential cross sections (DCS) for SF₆ and UF₆ at energies between 5 and 75 eV, and scattering angles of 20° to 135°. In Sec. II the instrument and the precautions taken for handling the corrosive and highly reactive UF₆ will be described. Since the details of the measurement technique have already been given in Ref. 1, only a brief description will be included here. The results and conclusions will be presented in Sec. III.

II. APPARATUS AND METHOD

Details of the experimental arrangement have been given in Refs. 1 and 2. Briefly, the apparatus consists of an electron gun which produces a collimated, energy-selected beam of electrons of impact energy E_0 . The electron beam crosses a target beam of the gas under investigation. This target beam is obtained by flowing the gas through a capillary array. Electrons scattered through a solid angle $d\Omega$ ($\approx 10^{-3}$ sr) at an angle θ with respect to the incident electron beam are energy analyzed and detected with a spiraltron electron multiplier. A multichannel analyzer is used to record the feature corresponding to elastically scattered electrons. The energy resolution employed in the present measurements was about 80 meV (FWHM). The rotational and vibrational-rotational transitions are, there-

fore, not resolved from pure elastic scattering. The intensity of elastic scattering is obtained by integrating the area under the elastic peak.

The method employs a measurement of the ratio of the intensity of the elastically scattered electrons by the gas under experimental investigation (SF₆ or UF₆) to that of He. This ratio is related to the ratio of cross sections $\sigma_{\text{exp}}(\theta)/\sigma_{\text{He}}(\theta)$ by the following relations:

$$\sigma_{\text{exp}}(\theta)/\sigma_{\text{He}}(\theta) = [\dot{N}_e(\text{exp})/\dot{N}_e(\text{He})] \times [m(\text{He})/m(\text{exp})]^{1/2} [\dot{N}_b(\text{He})/\dot{N}_b(\text{exp})], \quad (1)$$

or,

$$\sigma_{\text{exp}}(\theta)/\sigma_{\text{He}}(\theta) = [\dot{N}_e(\text{exp})/\dot{N}_e(\text{He})] [p(\text{He})/p(\text{exp})], \quad (2)$$

where $\sigma_{\text{exp}}(\theta)$ and $\sigma_{\text{He}}(\theta)$ are the DCS at an angle θ for the gas under experimental investigation (σ_{SF_6} or σ_{UF_6}) and for He, respectively, $\dot{N}_e(\text{exp})$ and $\dot{N}_e(\text{He})$ the experimentally measured intensities of the scattered electrons, $m(\text{He})$ and $m(\text{exp})$ the molecular weights, $\dot{N}_b(\text{He})$ and $\dot{N}_b(\text{exp})$ the flow rates into the scattering chamber as measured by gas flow meters, and $p(\text{He})$ and $p(\text{exp})$ the pressures behind the capillary array. These quantities and the derivations of Eqs. (1) and (2) are described in detail in Ref. 1. By this method we obtain the ratio of the differential cross section for the experimental gas to that of He. The absolute value of $\sigma_{\text{exp}}(\theta)$ is calculated by multiplying this ratio by the absolute value of $\sigma_{\text{He}}(\theta)$. Thus He DCS are used as secondary standards. However, for reasons of convenience, we measured σ_{UF_6} relative to N₂ DCS $\sigma_{\text{N}_2}(\theta)$. Since $\sigma_{\text{N}_2}(\theta)/\sigma_{\text{He}}(\theta)$ were known from our previous³ measurements, these ratios were then converted to $\sigma_{\text{UF}_6}/\sigma_{\text{He}}$.

As has been done for all the previously reported measurements,^{1,3,4} the following precautions were taken to reduce the possible sources of errors:

- (1) The energy of the incident electron beam was calibrated using the 19.35 eV resonance in He.
- (2) The true zero scattering angle was determined from the symmetry of the scattering intensity corresponding to the 2¹P excitation in He.
- (3) The incident electron beam was monitored by a Faraday cup for recording any change in the current during the course of the experiment.

(4) The contribution of the background scattering (both direct beam contribution and scattering by the background gas) to the scattering by the main molecular beam was measured by providing an alternate leak to the vacuum chamber. The flow to the chamber was switched from the capillary array to the alternate gas inlet and the proper background for the desired gas was established. At an energy E_0 , the angular distribution of the elastically scattered electrons was then measured. It was found that, for both gases above 20° scattering angle, the background scattering was negligible relative to scattering by the main beam under similar experimental conditions.

The gas handling schemes for UF_6 were different from SF_6 . The slight radioactivity of UF_6 served as a convenient property for monitoring the level of contamination. Of greater concern was the high chemical reactivity of UF_6 which necessitated the following special precautions:

(1) The molecular beam of UF_6 formed by the capillary array was directed into the mouth of a liquid nitrogen trap which captured a large fraction of the UF_6 beam.

(2) The small fraction of UF_6 that escaped from the primary liquid N_2 trap was captured by the liquid N_2 trap above the mercury diffusion pump and by a zeolite trap and third liquid N_2 trap located in the foreline of the mechanical pump. By this procedure the mechanical pump oil was protected from UF_6 . The mercury diffusion pump functioned well under these conditions but after the completion of the experiments the mercury was properly disposed of.

(3) At the completion of the experiment all UF_6 deposits were distilled over into a liquid nitrogen cooled collector by letting the UF_6 deposits warm up to room temperature.

(4) The electron optics were differentially pumped relative to the main scattering chamber.² The ambient pressure in the optics region was about 10^{-6} Torr for a main chamber pressure of 10^{-5} Torr. This feature probably allowed for longer experimental operation than would otherwise be possible.

(5) All materials which came into contact with the gases were made of either stainless steel or teflon.

Despite these precautions, after several weeks of experiment the electron optical elements were so badly contaminated that we were unable to observe the 19.35 eV He resonance at 90° . Under normal conditions one observes a 60% attenuation in the scattering intensity at this resonance.

III. RESULTS AND DISCUSSION

The ratios of $\sigma(\Theta)$ for SF_6 and UF_6 to those of He are presented in Tables I and II, respectively. The absolute values of $\sigma(\Theta)$ for these gases have been obtained by multiplying these ratios by the He cross sections of McConkey and Preston⁵ which are the only experimental results presently available for the energy range of interest here. However, the angular range reported by McConkey and Preston extends from 20° to 90° . Therefore, relative He cross sections in the 90° to 135° range were measured in our laboratory. The results and the details of the method employed for obtaining the

TABLE I. The ratios $\sigma_{\text{SF}_6}(\Theta)/\sigma_{\text{He}}(\Theta)$ at indicated scattering angles Θ and incident electron energies E_0 .

E_0 (eV) \ Θ (deg)	5	10	15	20	30	40	50	60	75
20	8.99	15.07	11.70	7.84	15.89	12.27	11.45	8.98	8.10
25	7.92	12.92	10.28	6.00	8.89	8.79	7.81	7.42	7.45
30	7.64	11.22	8.96	4.39	5.23	6.00	5.61	6.99	8.37
35	7.46	9.83	6.67	3.23	3.73	4.53	5.00	8.33	8.61
40	8.33	8.19	4.67	2.61	3.05	4.31	5.73	8.25	7.84
45	8.72	7.09	3.62	2.18	3.00	5.00	5.37	6.86	6.88
50	7.81	5.18	2.99	2.48	4.27	5.61	5.24	6.25	5.94
55	6.96	3.92	2.57	3.04	6.00	5.94	5.14	5.31	5.23
60	5.67	3.20	2.96	4.06	5.61	6.06	4.96	4.69	4.47
65	4.40	3.08	3.82	5.50	5.18	4.30	3.60	4.29	4.37
70	3.22	2.79	4.46	6.84	4.39	3.27	2.50	4.02	4.26
75	2.55	3.76	5.26	6.89	3.78	2.38	1.88	3.85	3.96
80	2.21	4.17	4.94	6.01	3.31	2.00	2.21	4.11	4.39
85	2.21	4.51	4.47	5.33	2.80	1.91	2.94	5.16	5.00
90	2.32	4.31	3.96	4.27	2.54	2.12	4.19	6.00	5.94
95	2.40	3.71	3.43	3.47	2.72	2.75	4.66	6.98	5.52
100	2.60	3.23	3.30	3.37	3.28	3.89	5.19	7.60	5.19
105	2.71	2.69	2.47	2.50	3.59	4.62	5.45	5.92	6.15
110	2.79	2.19	2.40	2.91	4.42	5.95	5.74	5.80	8.00
115	2.54	1.78	2.26	3.04	5.00	6.84	5.89	6.60	10.00
120	2.38	1.62	2.27	3.23	5.54	8.00	7.12	7.13	12.31
125	1.98	1.78	2.11	2.96	5.73	8.67	8.18	8.73	15.71
130	1.65	1.71	2.37	3.40	6.38	9.69	9.72	11.67	20.67
135	1.37	2.17	2.83	4.32	8.06	10.70	14.73	21.88	26.25

TABLE II. The ratios $\sigma_{\text{UF}_6}(\Theta)/\sigma_{\text{H}_2}(\Theta)$ at indicated scattering angles Θ and incident electron energies E_0 .

Θ (deg) \ E_0 (eV)	10	15	20	30	40	50	60	75
20	11.54	18.62	33.98	111.87	21.87	26.26	17.39	9.97
25	10.00	15.55	22.86	11.11	9.39	10.94	6.77	9.80
30	8.01	12.43	13.64	8.46	5.00	7.54	7.17	9.07
35	7.96	10.00	8.38	6.10	5.47	7.80	7.50	7.78
40	6.10	7.01	5.57	5.53	6.25	8.94	7.04	6.86
45	5.40	5.52	4.26	5.63	6.19	7.37	5.60	5.92
50	3.70	4.41	4.36	5.68	6.15	6.10	4.44	5.35
55	2.83	3.67	5.00	5.50	5.21	4.86	3.59	4.88
60	2.00	3.61	5.89	4.81	4.79	4.44	3.56	4.61
65	1.67	4.36	6.75	4.35	5.16	5.30	5.10	4.53
70	1.49	5.58	7.22	3.66	5.90	6.02	4.37	4.63
75	1.52	6.36	7.50	3.24	5.14	5.75	3.59	4.79
80	1.59	6.01	6.99	3.02	4.74	4.94	2.88	5.36
85	1.59	5.87	6.11	2.72	4.04	3.97	2.74	6.39
90	1.65	5.21	4.95	2.62	3.65	3.06	2.91	7.19
95	1.60	4.64	4.53	3.12	3.75	3.45	3.21	8.28
100	1.48	3.80	3.67	4.05	4.17	3.89	3.60	10.37
105	1.34	3.27	2.90	3.91	4.10	4.18	4.49	12.69
110	1.22	3.18	3.13	4.33	4.73	5.74	6.40	16.40
115	1.13	2.80	3.14	4.52	5.26	8.93	10.60	20.40
120	1.09	2.74	3.28	4.92	7.25	12.54	15.09	23.08
125	1.03	2.70	3.12	5.33	9.11	16.67	20.00	26.43
130	0.90	3.29	3.40	6.25	11.46	19.44	22.50	28.67
135	0.93	4.99	4.73	8.71	14.89	22.97	24.22	29.38

TABLE III. SF_6 differential elastic cross sections $\sigma(\Theta)$, ($10^{-20}\text{m}^2/\text{sr}$). The percentages contributed by the extrapolations of $\sigma(\Theta)$ between 0° and 20° and between 135° and 180° to the elastic integral and momentum transfer cross sections are shown in parentheses.

Θ (deg) \ E_0 (eV)	5	10	15	20	30	40	50	60	75
20	2.05	4.90	4.40	2.90	6.20	4.60	4.10	3.10	2.60
25	1.90	4.20	3.70	2.10	3.20	2.90	2.50	2.30	1.90
30	1.85	3.50	3.10	1.45	1.70	1.80	1.60	1.90	1.80
35	1.85	2.90	2.20	1.00	1.10	1.20	1.25	2.00	1.55
40	2.00	2.35	1.50	0.75	0.80	1.00	1.25	1.70	1.20
45	2.05	1.95	1.05	0.59	0.74	1.05	1.02	1.20	0.86
50	1.85	1.40	0.78	0.62	0.94	1.05	0.86	0.90	0.60
55	1.60	1.02	0.63	0.70	1.20	0.98	0.72	0.68	0.45
60	1.35	0.80	0.69	0.86	1.05	0.86	0.58	0.54	0.34
65	1.10	0.77	0.84	1.10	0.88	0.55	0.36	0.42	0.28
70	0.85	0.82	1.00	1.28	0.72	0.36	0.22	0.35	0.23
75	0.70	0.94	1.20	1.24	0.56	0.25	0.15	0.30	0.19
80	0.62	1.05	1.15	1.10	0.46	0.19	0.17	0.30	0.18
85	0.64	1.15	1.05	0.96	0.37	0.17	0.20	0.32	0.18
90	0.69	1.15	0.95	0.82	0.33	0.18	0.26	0.33	0.19
95	0.75	1.02	0.85	0.66	0.34	0.22	0.27	0.37	0.16
100	0.86	0.94	0.76	0.57	0.38	0.28	0.28	0.38	0.14
105	0.95	0.82	0.68	0.50	0.46	0.36	0.30	0.29	0.16
110	1.05	0.72	0.62	0.53	0.53	0.44	0.31	0.29	0.20
115	1.05	0.63	0.63	0.58	0.62	0.52	0.33	0.33	0.25
120	1.02	0.61	0.68	0.65	0.72	0.64	0.42	0.38	0.32
125	0.95	0.71	0.78	0.74	0.86	0.78	0.54	0.48	0.44
130	0.86	0.82	0.89	0.90	1.02	0.93	0.70	0.70	0.62
135	0.78	1.05	1.05	1.05	1.25	1.01	1.09	1.40	0.84
Integral (10^{-20}m^2)	14 (16%)	17 (26%)	16 (30%)	14 (36%)	17 (47%)	14 (48%)	13 (54%)	15 (53%)	9.0 (46%)
Mom. transfer (10^{-20}m^2)	11 (19%)	12 (34%)	13 (41%)	13 (43%)	13 (49%)	11 (56%)	11 (63%)	15 (71%)	6.8 (57%)

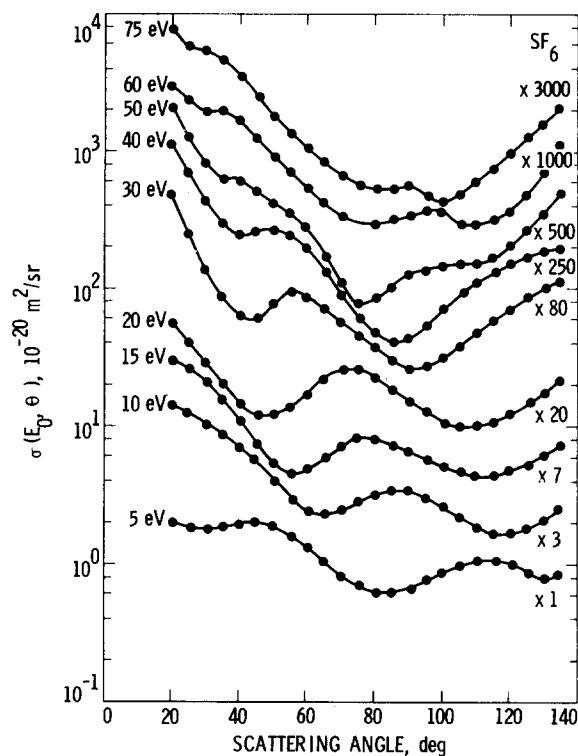


FIG. 1. Elastic DCS for SF_6 at several electron impact energies. The true value of the cross section is obtained by dividing the number on the y axis by the multiplication factor shown on the right hand corner of each curve. Solid lines are interpolations between the experimental data.

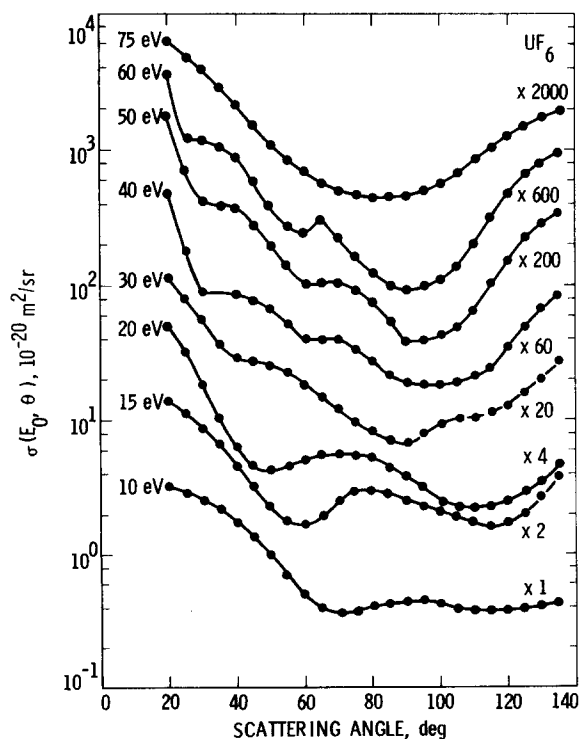


FIG. 2. Elastic DCS for UF_6 at several electron impact energies. The true value of the cross section is obtained by dividing the number on the y axis by the multiplication factor shown on the right hand corner of each curve. Solid lines are interpolations between the experimental data.

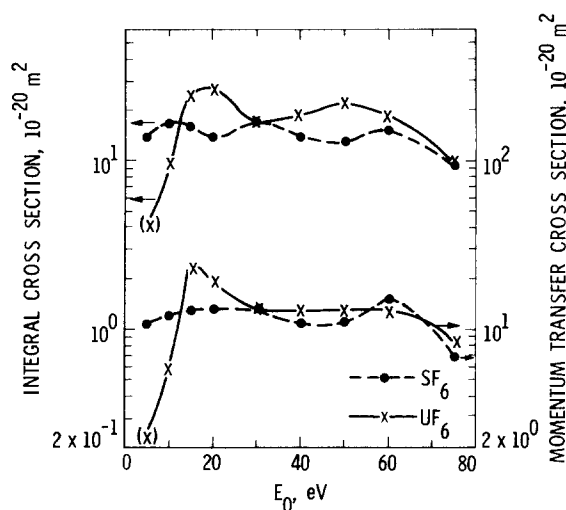


FIG. 3. Elastic integral and momentum transfer cross sections for SF_6 and UF_6 . Upper curves to be read on the left hand ordinate and the lower ones on the right hand ordinate. Solid lines are interpolations between the experimental data. The 5 eV points for UF_6 were obtained from the extrapolated DCS's of Table IV.

absolute values will be presented in a future publication.⁶

Tables III and IV give the absolute values of elastic DCS for SF_6 and UF_6 , respectively. In Figs. 1 and 2 the angular distribution curves are plotted. In these curves two shallow minima are present which shift gradually toward smaller scattering angles with increasing impact energy.

The ratios $\sigma_{\text{SF}_6}(\theta)/\sigma_{\text{He}}(\theta)$ or $\sigma_{\text{UF}_6}(\theta)/\sigma_{\text{He}}(\theta)$ are measured by utilizing either Eq. (1) or (2). Therefore, the errors are dependent on the accuracies with which the quantities on the right hand side of these equations can be measured. These errors have been estimated and the details are given in Table II of Ref. 1. For SF_6 , the ratios $\sigma_{\text{SF}_6}(\theta)/\sigma_{\text{He}}(\theta)$ are estimated to be accurate to within $\pm 10\%$. The estimated error for $\sigma_{\text{UF}_6}(\theta)/\sigma_{\text{He}}(\theta)$ is about $\pm 33\%$. This large error is mainly due to the change of incident electron beam current when He is replaced by UF_6 . During the course of the experiment, it was found that UF_6 affected the electron optics even though the optical system was differentially pumped. The errors in the absolute values of $\sigma_{\text{SF}_6}(\theta)$ and $\sigma_{\text{UF}_6}(\theta)$ given in Tables III and IV are $\pm 15\%$ and $\pm 35\%$, respectively. This error is a root sum of squares of individual errors in the ratios of cross sections and a $\pm 12\%$ error⁵ in the absolute values of $\sigma_{\text{He}}(\theta)$.

The error in the shapes of the angular distribution curves, on the other hand, depends on the errors in the relative value of both $\sigma_{\text{exp}}(\theta)/\sigma_{\text{He}}(\theta)$ and $\sigma_{\text{He}}(\theta)$. It is evident from Table II of Ref. 1 that the error in the relative values of $\sigma_{\text{exp}}(\theta)/\sigma_{\text{He}}(\theta)$ is only $\pm 2\%$. The error in the relative values⁵ of $\sigma_{\text{He}}(\theta)$ is approximately $\pm 11\%$. Therefore, the error in the shapes of curves shown in Figs. 1 and 2 is about $\pm 11\%$ for both SF_6 as well as UF_6 which is a root sum of squares of individual errors.

In order to obtain elastic integral and momentum

TABLE IV. UF_6 differential elastic cross sections $\sigma(\theta)$, ($10^{-20} m^2/sr$). The percentages contributed by the extrapolations of $\sigma(\theta)$ between 0° and 20° and between 135° and 180° to the elastic integral and momentum transfer cross sections are shown in parentheses. The data reported here for the 5 eV electron impact energy have been obtained by extrapolating $\sigma(\theta)$ values at other energies.

E_0 (eV) θ (deg)	5	10	15	20	30	40	50	60	75
20	1.60	3.75	7.00	12.50	5.80	8.20	9.40	6.00	3.20
25	1.30	2.90	5.60	8.00	4.00	3.10	3.50	2.10	2.50
30	1.20	2.50	4.30	4.50	2.75	1.50	2.15	1.95	1.95
35	1.10	2.15	3.30	2.60	1.80	1.45	1.95	1.80	1.40
40	0.88	1.75	2.25	1.60	1.45	1.45	1.95	1.45	1.05
45	0.70	1.35	1.60	1.15	1.35	1.30	1.40	0.98	0.74
50	0.52	1.00	1.15	1.09	1.25	1.15	1.00	0.64	0.54
55	0.34	0.68	0.90	1.15	1.10	0.86	0.68	0.46	0.42
60	0.25	0.50	0.84	1.25	0.90	0.68	0.52	0.41	0.35
65	0.16	0.40	0.98	1.35	0.74	0.66	0.53	0.50	0.29
70	0.16	0.37	1.25	1.35	0.60	0.65	0.53	0.38	0.25
75	0.16	0.38	1.45	1.35	0.48	0.54	0.46	0.28	0.23
80	0.20	0.40	1.40	1.28	0.42	0.45	0.38	0.21	0.22
85	0.18	0.43	1.38	1.10	0.36	0.36	0.27	0.17	0.23
90	0.18	0.44	1.25	0.95	0.34	0.31	0.19	0.16	0.23
95	0.18	0.44	1.15	0.86	0.39	0.30	0.20	0.17	0.24
100	0.18	0.43	0.95	0.62	0.47	0.30	0.21	0.18	0.28
105	0.15	0.41	0.90	0.58	0.50	0.32	0.23	0.22	0.33
110	0.13	0.40	0.82	0.57	0.52	0.35	0.31	0.32	0.41
115	0.11	0.40	0.78	0.60	0.56	0.40	0.50	0.53	0.51
120	0.12	0.41	0.82	0.66	0.64	0.58	0.74	0.80	0.60
125	0.11	0.41	1.00	0.78	0.80	0.82	1.10	1.10	0.74
130	0.11	0.43	1.30	0.90	1.00	1.10	1.40	1.35	0.86
135	0.12	0.45	1.85	1.15	1.35	1.40	1.70	1.55	0.94
Integral ($10^{-20} m^2$)	4.3 (23%)	9.6 (25%)	25 (39%)	27 (43%)	17 (43%)	19 (55%)	22 (59%)	18 (60%)	9.5 (38%)
Mom. transfer ($10^{-20} m^2$)	2.4 (27%)	5.9 (32%)	24 (55%)	19 (46%)	13 (54%)	13 (58%)	13 (55%)	13 (57%)	8.0 (47%)

transfer cross sections, the angular distribution curves shown in Figs. 1 and 2 were extrapolated between 0° and 20° and between 135° and 180° . Since no guide was available for this extrapolation, between 0° and 20° a straight line was drawn whose slope was determined by the data between 20° and 30° . A similar extrapolation was done for the region between 135° and 180° with the slope given by the data between 115° and 135° . In Tables III and IV, these cross sections are shown at the bottom of each column. The percentage contributed by the extrapolation regions are shown in parentheses. These quantities give an idea of the extent of possible error in the extrapolations. We estimate that the errors in the elastic integral and momentum cross sections for SF_6 are $\pm 18\%$ and $\pm 20\%$, respectively. For UF_6 , these quantities have been estimated to be $\pm 40\%$ and $\pm 45\%$, respectively.

In Fig. 3 are shown the elastic integral and momentum transfer cross sections for SF_6 and UF_6 at several electron impact energies. It is evident from these curves that both gases, above 10 eV impact energy,

have similar cross sections, but they differ from each other at low energies. Both SF_6 and UF_6 have higher elastic integral and momentum transfer cross sections than H_2 , especially at higher energies.

*Supported in part by the National Aeronautics and Space Administration under Contract No. NAS7-100 to the Jet Propulsion Laboratory and in part by ERDA Order No. LS-76-5.

[†] Some of the results reported here were presented at the ninth ICPEAC, Seattle, Washington, July 24-30, 1975.

¹ S. K. Srivastava, A. Chutjian, and S. Trajmar, *J. Chem. Phys.* **63**, 2659 (1975).

² A. Chutjian, *J. Chem. Phys.* **61**, 4279 (1974).

³ S. K. Srivastava, A. Chutjian, and S. Trajmar, *J. Chem. Phys.* **64**, 1340 (1976).

⁴ S. K. Srivastava, S. Trajmar, A. Chutjian, and W. Williams, "Electronic and Atomic Collisions" abstracts of papers of the ninth International Conference on the Physics of Electronic and Atomic Collisions, edited by John S. Risley and R. Geballe, p. 265.

⁵ J. W. McConkey and J. A. Preston, *J. Phys. B* **8**, 63 (1975).

⁶ S. K. Srivastava and S. Trajmar, *J. Chem. Phys.* (to be published).