

# GENERALIZED OSCILLATOR STRENGTHS

## Progress Report

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### ABSTRACT

Collision cross section determinations on the transition  $E^3 \Sigma_g^+ \leftarrow X^1 \Sigma_g^+$  in  $N_2$  at 100, 200, and 300 eV show that the cross section decreases steadily at each kinetic energy as the scattering angle increases at angles in the range  $2^\circ \longrightarrow 14^\circ$ . Thus, the transition resembles the  $2^3S \leftarrow 1^2S$  transition helium studied by Dillon [J. Chem. Phys. 63, 2035 (1975)]. Both singlet-triplet transitions belong to a class for which the cross section is abnormally high in forward scattering as expected, since the orbital term symbol is the same in ground and excited states. The study of the singlet-triplet transition in  $N_2$  is continuing.

Two theoretical studies have been completed, one on the functional form at one-electron momentum distributions deduced from a local one-electron potential function, and the second on the connection between generalized oscillator strengths and collision cross sections (in Born approximation) for resonant energy transfer in the collision of two molecules.

Modifications in the collision cell and electrostatic lens system of an electron spectrometer are planned. A new pressure gauge, which extends accurate pressure measurements in the collision cell to pressures lower by tenfold, has been installed and is in use.

## 1. INTRODUCTION

The following progress report is organized with the same section numbers as the proposal submitted last year, so that the status of each item is clearly and specifically stated. There are two exceptions. Section 2.6 describes two researches, in sub-sections 2.61 and 2.62, which were not proposed last year. The cross section study of Section 2.5 occupied the electron spectrometer so completely that other researches using that instrument could not be done. Hence, the two theoretical researches were undertaken and are described in Section 2.6. One is completed and a manuscript has been accepted for publication. The second is being continued under other auspices. (See Section 2.62.)

## 2. RESEARCH PROGRAM

### 2.1 Pressure Measurement.

Polyatomic molecules are such strong scatterers that multiple collisions are important unless lower pressures or shorter path lengths (or both) can be used. To obtain lower pressures, a more sensitive pressure gauge is necessary. Installation of a new pressure gauge was proposed for the current contract period. An improved version of the capacitance manometer (MKS Instrument Co.) was purchased and installed. After extensive testing and development, the first pressure head was found to be unsatisfactory because of excessive noise. A second head, of different design, was tried and found to be satisfactory. Pressures as low as 0.01 micron ( $1 \times 10^{-5}$  Torr) can be measured with an accuracy of about 5%. The gauge is more sensitive by a factor of ten than the gauge previously used. Its performance is satisfactory. No further changes are needed and none are planned.

### 2.2 Modification of Collision Cell

Modification of the collision cell (to shorten path length of electrons through the scattering gas and reduce multiple collisions) has been delayed pending completion of the cross section study on the transition  $E^3\Sigma_g^+ \leftarrow X^1\Sigma_g^+$  in  $N_2$  (see Section 2.5). When this modification is made, the electrostatic lens system between monochromator and collision cell will also be changed. See accompanying renewal proposal.



### 2.3 Continuing and Incomplete Studies

The investigation of  $\text{H}_2\text{O}$  is completed and published [K. N. Klump and E. N. Lassette, Can. J. Phys. 53, 1825 (1975)]. No additional research is planned.

The experimental study of  $\text{CO}_2$  is finished. A manuscript has not been prepared as yet, but this will be done as soon as time permits.

No further research has been done on benzene but strong reasons have developed for determining generalized oscillator strengths on a (weak) vibronically allowed transition in benzene and another in acetone. This is discussed in an accompanying proposal.

For discussion of the singlet-triplet collision cross section study on  $\text{N}_2$ , see Section 2.5 below.

### 2.4 Search for Singlet-Triplet Transitions with Same Term Symbols in Ground and Excited States Electron Impact Spectra

A search for new singlet-triplet transitions, with the same term symbols in ground and excited states, was proposed during the present contract period. Polyatomic substances ( $\text{CH}_3\text{F}$ , Propylene, unsymmetrically substituted ketanes and aldehydes) were to be employed. This study has been deferred pending completion of the singlet-triplet collision cross section study described in Section 2.5 below.

### 2.5 Collision Cross Section Studies

It was proposed last year that electron collision cross sections for the transition  $E^3\Sigma_g^+ \leftarrow X^2\Sigma_g^+$  in  $\text{N}_2$  should be deter-

mined over the initial electron kinetic energy range 25-500 eV.

This cross section study is still in progress but is nearing completion, as described below.

Simultaneous with the determination of collision cross sections, an extensive exploration of the limits of kinetic energy capability of the electron spectrometer was undertaken. It was necessary to do this since we are now aiming at quantitative collision cross section determinations, whereas the last exploration of this type was done to establish the limits within which electron impact spectra can be obtained, a less demanding application. This exploration was very time consuming because the cross section study, on the singlet-triplet transition mentioned above, is the most difficult that we have ever undertaken both because of low intensities and because the transition of interest is superimposed on another whose relative intensity changes with both scattering angle and kinetic energy of incidence. The investigation showed that relative intensities can be determined quantitatively between 50 eV and 300 eV incident kinetic energy. With the recent spectrometer configuration quantitative determinations on the singlet-triplet transition could not be done at kinetic energies below 50 eV. The upper limit, 300 eV, applies only to the singlet-triplet transition. More intense transitions can be, and have been, studied at kinetic energies up to 600 eV and higher kinetic energies could be used after some minor modifications. Cross section studies at lower kinetic energies require modification of the electrostatic lens system between monochromator and collision cell. This point is discussed later.

The singlet-triplet transition under consideration occurs at an energy loss of 11.87 eV. The transition  $a''^1\Sigma_g^+ \leftarrow x^1\Sigma_g^+$  is the corresponding singlet-singlet transition and occurs at an energy loss of 12.26 eV. The behavior of these two transitions with change in scattering angle at three different kinetic energies of incidence, 50 eV, 100 eV and 200 eV are shown in Figures 1, 2, and 3, respectively. The two transitions of interest are apparent at the extreme right of each figure. The transition at 11.87 eV is superimposed on other, less intense, transitions which appear as a "background" which must be subtracted off in cross section determinations. Designate the cross section for the singlet-triplet transition by  $\sigma_T$ , that for the singlet-singlet transition by  $\sigma_S$ , and the cross section for elastic scattering by  $\sigma_e$ . Then it is the usual procedure to first determine the ratio  $\sigma_T/\sigma_S$ . Then the ratio  $\sigma_S/\sigma_e$  is determined in cases where the elastic cross section is known. Then from the ratio  $\sigma_S/\sigma_e$  and the value of  $\sigma_e$  the value of  $\sigma_S$  can be obtained.  $\sigma_T$  is found from the ratio  $\sigma_T/\sigma_S$ .

A singlet-triplet transition for which the orbital term symbol is the same in ground and excited state has abnormally high cross section at small scattering angles and high kinetic energy. This, at least, is the hypothesis which is being experimentally tested. Obviously, high kinetic energy and small scattering angle must be employed in testing the hypothesis, and this is the primary source of difficulty. For the transition is weak (relative to other singlet-singlet transitions) and hence large angular apertures are essential.

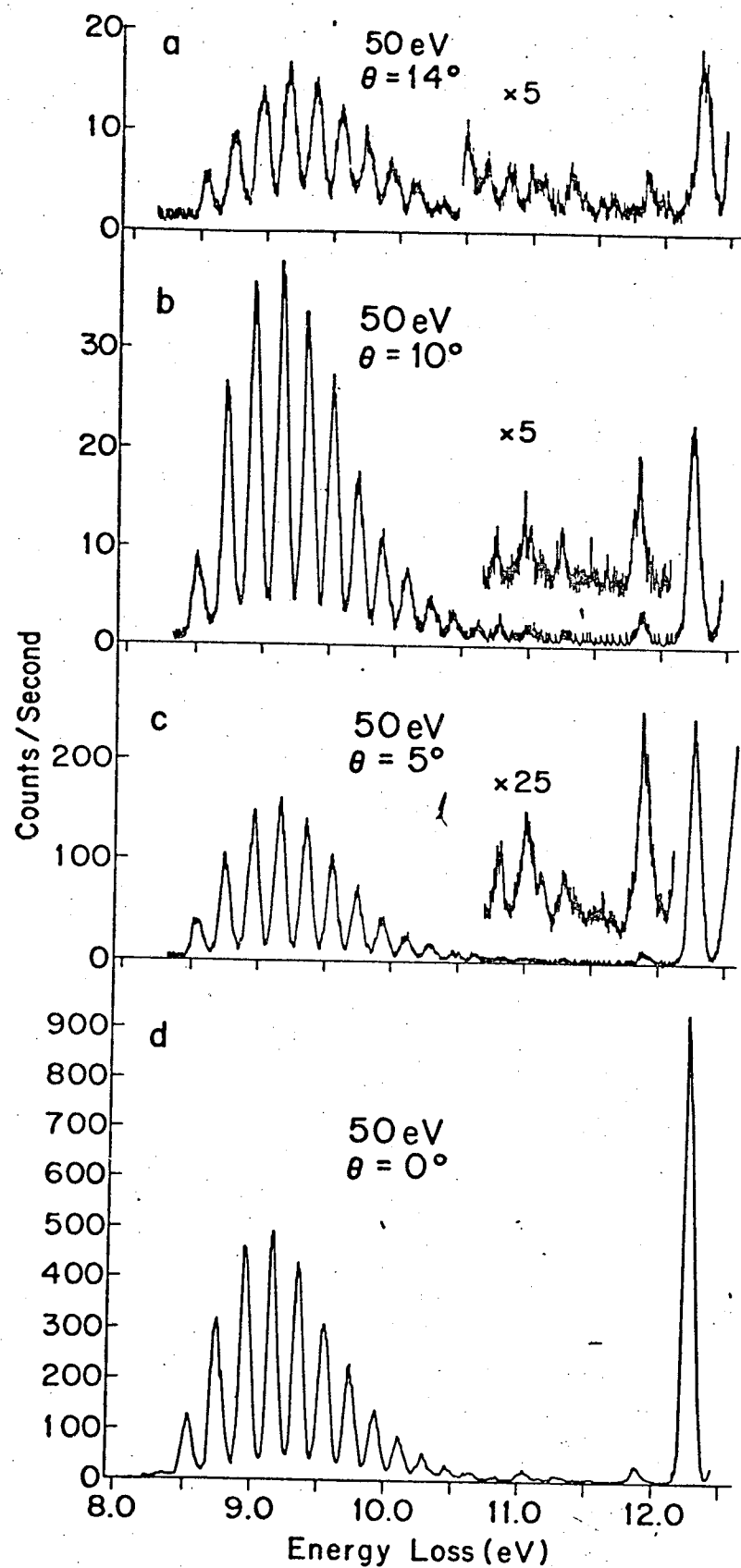


FIG. 1 Electron energy loss spectra of  $N_2$ . Energy of incident electrons is 50 eV. Scattering angle,  $\theta$ , is (a)  $14^\circ$ , (b)  $10^\circ$ , (c)  $5^\circ$ , (d)  $0^\circ$ .

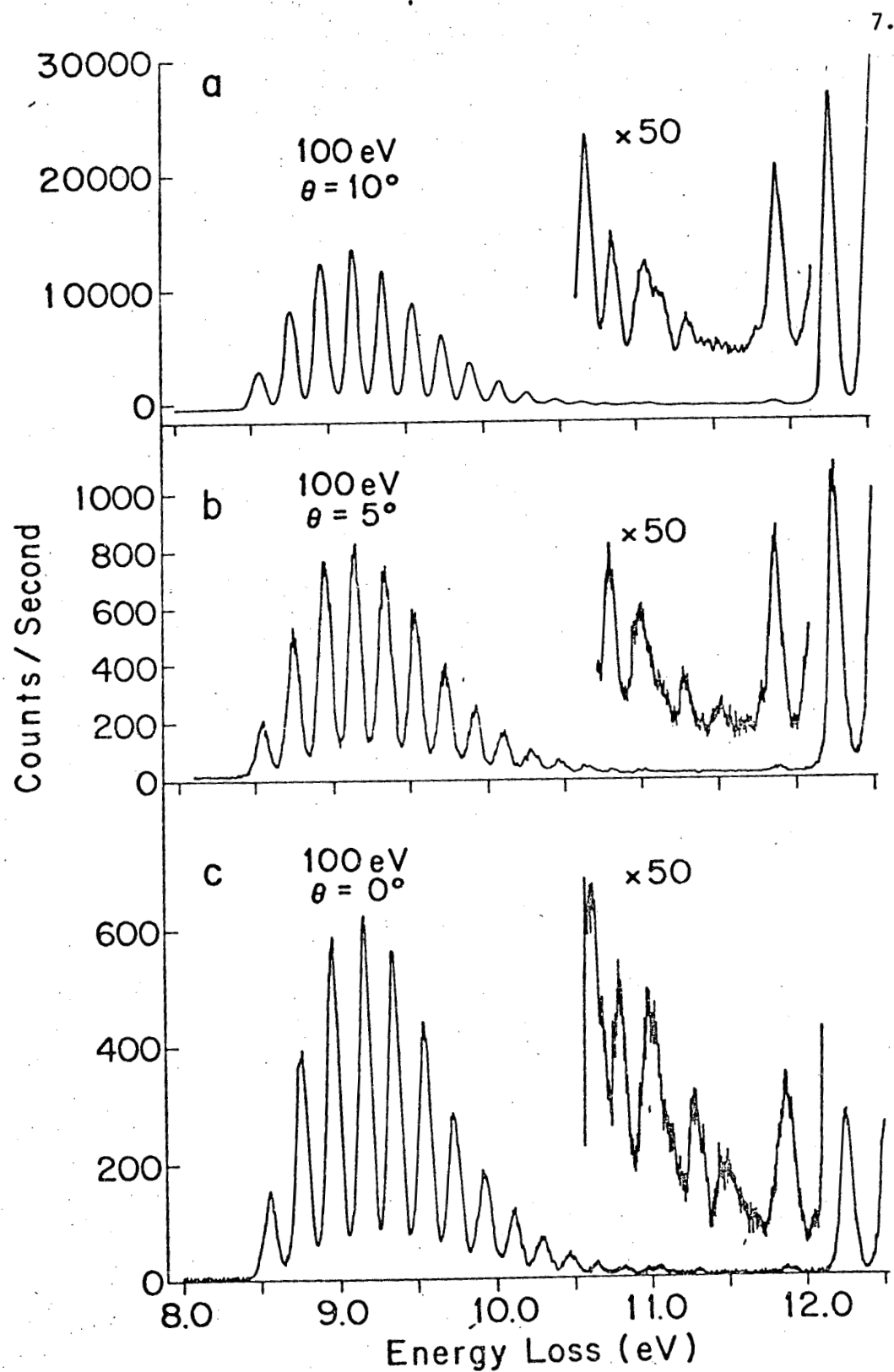


FIG. 2 Electron energy loss spectra of  $N_2$ . Energy of incident electrons is 100 eV. Scattering angle is (a)  $10^\circ$ , (b)  $5^\circ$ , (c)  $0^\circ$ .

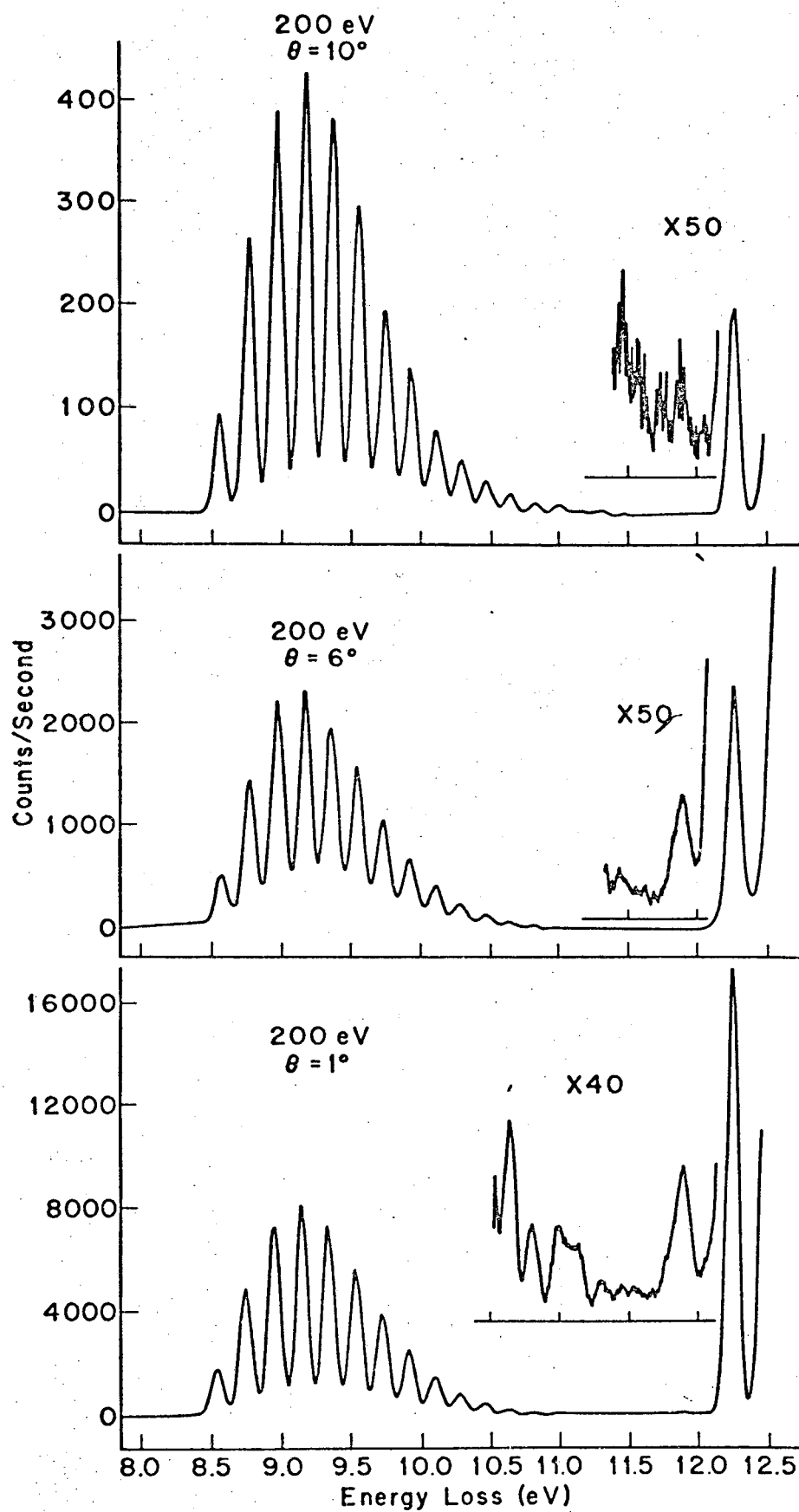


FIG. 3 Electron energy loss spectra of  $N_2$ . Energy of incident electrons is 200 eV.

This not only introduces ~~maximum~~ uncertainty at small scattering angle (precisely the region of greatest interest) but even more important the reproducibility at small scattering angle is poor because such wide slits are employed that a change in intensity distribution in the incident electron beam gives rise to an apparent change in angle. Under these conditions, we must expect greater scatter in the cross section data than we have had in previous research.

Collision cross sections for the singlet-triplet transition, obtained to date, are shown in Table 1. At each kinetic energy, the cross section decreases steadily with increase in scattering angle. This is qualitatively similar to the behavior found by Dillon [J. Chem. Phys. 63, 2035 (1975)] for the transition  $2^3S \leftarrow 1^1S$  in helium over the same range of scattering angle. Hence, the abnormal behavior of the singlet-triplet transition in nitrogen is confirmed. The term "abnormal" is used as a contrast to the behavior expected from the first Born approximation with exchange (Born-Oppenheimer approximation). At 50 eV only the ratio  $\sigma_T/\sigma_S$  has been determined. This is shown in Fig. 4. The ratio  $\sigma_S/\sigma_e$  was also measured, but we have no elastic cross section at this kinetic energy and hence  $\sigma_T$  cannot yet be calculated. Other methods of calibrating, not requiring elastic cross sections, are under consideration but have not yet been used. The cross sections at 300 eV in Table 1 are subject to large errors. Additional determinations on these quantities will be done. (See Section 3.)

TABLE 1

N<sub>2</sub>: Cross-sections for E<sup>3</sup> Σ<sub>g</sub><sup>+</sup> ← X<sup>1</sup> Σ<sub>g</sub><sup>+</sup> Scattering Summary

$\theta$ (deg.) \ E <sub>0</sub> (eV)	$\sigma_T \times 10^4$ (Atomic Units)		
	100	200	300
2	--		40.4 ± 16.5
3	--		20.7 ± 7.2
4	--	8.44 ± 1.37	7.08 ± 1.48
5	24.8 ± 3.2	6.375 ± .977	5.59 ± 1.95
6	27.2 ± 6.7	4.736 ± .589	2.69 ± 1.97
7	17.60 ± 3.50	3.819 ± .504	2.61 ± 1.90
8	14.96 ± 1.37	2.442 ± .407	--
9	12.78 ± 1.49	1.743 ± .411	--
10	11.50 ± 1.46	1.181 ± .287	--
12	7.59 ± 1.45	0.533 ± .307	--
14	3.96 ± .72	--	--



## Nitrogen

Initial Kinetic Energy 50eV

 $\sigma_T / \sigma_S$  $10^{-1}$  $10^{-2}$ 

0

4

8

12

16

20

Scattering Angle

FIG. 4 The ratio of  $\sigma_T$  for the transition  $E^3 \Sigma_g^+ \leftarrow X^1 \Sigma_g^+$  to  $\sigma_S$  for the transition  $a''^1 \Sigma_g^+ \leftarrow X^1 \Sigma_g^+$ .

## 2.6 New Researches.

The singlet-triplet cross section studies described in Section 2.5 occupied the electron spectrometer completely for such long periods that no other experimental research could be done. Hence, two theoretical researches were initiated, one by E. N. Lassettre mentioned in Section 2.61 below and the second by Winifred M. Huo in Section 2.62 below. These were briefly described in an accompanying technical report covering the period January 1, 1970 to July 1, 1976. Essentially, the same account of each research is given in the following two sections.

### 2.61 Momentum Eigenfunctions.

An investigation of momentum eigenfunctions has been undertaken for two reasons. First, the mathematical methods used by others in the study of form factors can be applied with little or no modification to momentum eigenfunctions for atoms and molecules. Second, we need (for molecules) approximate eigenfunctions similar to Hartree-Fock functions for atoms in order to carry out approximate collision amplitude calculations to use in directing our experiment, especially on singlet-triplet transitions. Although quantum chemists have made impressive progress on energy calculations using Gaussian basis sets the eigenfunctions are never published and are almost completely inaccessible to us. Therefore, the problem of expressing the potential energy  $V$  of an electron in a molecule as a sum of atom centered potentials, using the potential function mentioned in Section 6.2, has been considered. Next,

we have considered the potential function  $U_n$  from which we can obtain atomic orbitals  $\phi_n$  which participate in linear combinations to form molecular orbitals  $\psi$

$$\psi = \sum_n C_n \phi_n$$

The function  $\phi_n$  satisfies a one-electron Schrödinger type equation

$$-1/2\nabla^2 \phi_n + U_n \phi_n = W_n \phi_n.$$

If successful in obtaining  $U_n$ , this equation could be integrated by conventional methods somewhat similar to the self consistent field procedure. It is possible to formulate this problem in a manner suitable for numerical calculation. This has been done, a manuscript has been prepared and accepted for publication. (Item 21 of the publication list.) Questions have arisen about the potential function which would require an investigation of many months duration, too long to be of value in the present project. Therefore, a proposal has been submitted to NSF for the support of a research program which is entirely theoretical. (See Section 4.) If the proposal is funded, the research will be resumed under NSF auspices. As far as the present research program is concerned, this investigation has been terminated.

#### 2.62 Resonant Energy Transfer Cross Sections. (Winifred M. Huo)

A typical energy transfer reaction takes place when an excited

molecule  $D'$  collides with  $A$  and excites it to  $A'$  while  $D'$  undergoes transition to a lower energy state  $D$  with energy evolution  $\Delta E$ , i.e.,



After some manipulation, which will be omitted, the Born approximation for the differential collision cross section can be put into the form

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_o} \frac{M_\mu^2}{W_A W_D} f_D f_A$$

where  $M_\mu$  is the reduced mass and

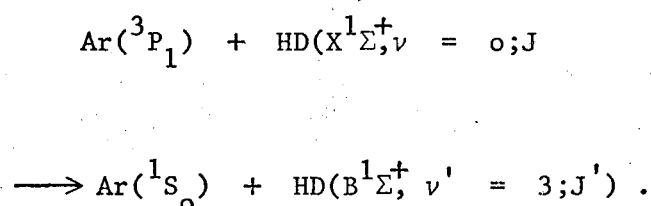
$$f_A = \frac{2W_A}{K^2} \left| \langle \psi_{A'} | \sum_j e^{i\vec{K} \cdot \vec{r}_{jA}} | \psi_A \rangle \right|^2$$

$$f_D = \frac{2W_A}{K^2} \left| \langle \psi_{D'} | \sum_j e^{i\vec{K} \cdot \vec{r}_{jD}} | \psi_D \rangle \right|^2.$$

In these formulas  $\vec{r}_{jA}$  represents the position vector of the  $j^{\text{th}}$  electron in molecule  $A$  and the summation extends over all electrons of molecule  $A$ . The eigenfunctions in the ground and excited states are  $\psi_A, \psi_{A'}$ . The corresponding quantities for molecule  $D$  are obvious. Also  $k_o$  and  $k_e$  are the initial and final (relative) momenta and  $W_A, W_D$  are the excitation energies. The vector  $\vec{K}$  is the relative momentum change of the center of mass of  $A$  in collision. That for  $D$  is  $-\vec{K}$ . The quantities  $f_A$  and  $f_D$  have precisely the same form as the generalized oscillator

strengths in electron molecule collisions but  $\mathbf{K}$  is now the momentum change of the colliding electron and  $k_o, k_f$  are the initial and final momenta. Because  $M_\mu$  is so much bigger than the mass of an electron the momentum change  $K$  accompanying the collision of molecules A and D' (to produce A' + D) covers about the same range for molecules in the thermal energy range as  $K$  does for molecule collisions with electrons having kinetic energies of hundreds of volts, just the region which we are studying experimentally. The fact that a collision cross section (in Born approximation) for molecule-molecule scattering is obtainable from generalized oscillator strengths obtained by electron-molecule scattering seems to us to be highly significant because it makes possible the precise determination of the cross section in Born approximation.

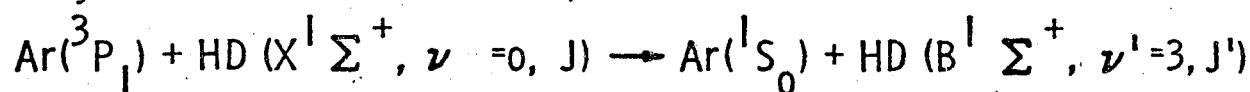
The importance of the formula for the Born cross section can be illustrated by considering the following reaction



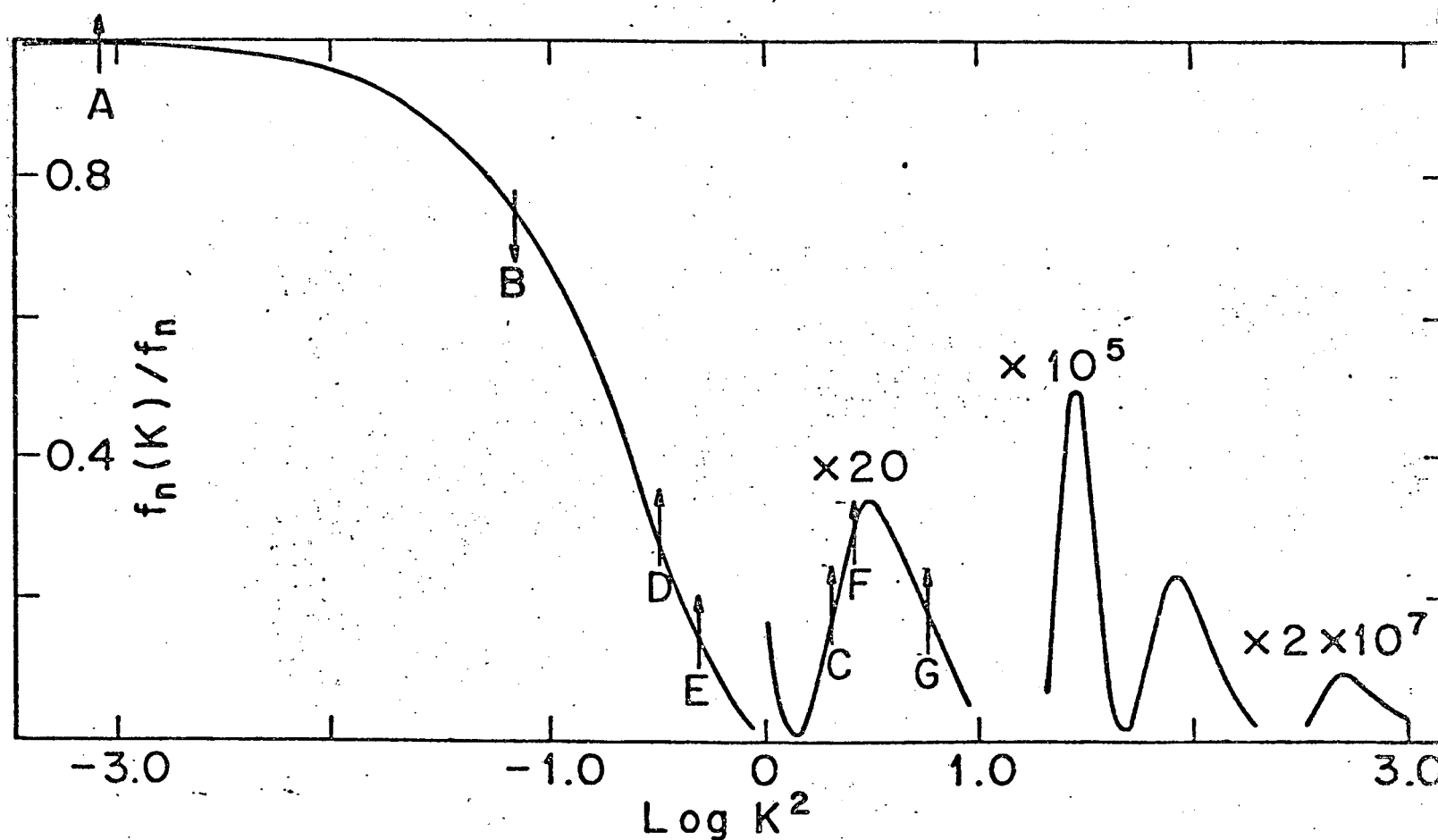
Relative cross sections have been measured by E. H. Fink, D. Wallach, and C. B. Moore [J. Chem. Phys. 56, 3608 (1972)] and made absolute by using the measured quenching cross section determinations of J. R. McNeely, C. S. Hurst, E. B. Wagner, and M. G. Payne [J. Chem. Phys. 63, 2717 (1975)]. The results are given in Table of Fig. 5 (see column 6). The collision cross section calculated from the above

Summary of results of the reaction at 300°K.

16.

Thermal averaged cross section ( $\text{\AA}^2$ )

Reaction #	J	J'	$\Delta E(\text{cm}^{-1})$	Calculated	Experimental	Calc/Exptl.
A	1	2	3.7	31.3	39.1	0.80
B	0	1	-34	11.3	14.1	0.81
C	2	1	233	0.06		
D	1	0	81	2.4	0.82	2.9
E	2	3	104	1.6	0.27	5.9
F	3	4	267	0.02	< 0.2	
G	4	5	492	0.0003	< 0.1	
				46.7	54.3	0.86



Relative generalized oscillator strength for the excitation of Ar.

R. Albat, N. Gruen, and W. Wirsam, J. Phys. B8, L82 (1975).

formulas, integrated over angle, and averaged over the thermal velocity distribution is given in column 5. The resonant energy gap,  $\Delta E$ , is given in column 4. To calculate the cross sections, the generalized oscillator strengths must be known. That for argon is given in Fig. 5. For hydrogen the shape of the oscillator strength curve was assumed to be given by the calculations of Miller and Krauss [J. Chem. Phys. 47, 3754 (1967)]. For both argon and hydrogen, the oscillator strength curves were normalized to give the correct (measured) optical oscillator strength. In the case of argon the state is labeled  $^3P_1$ . However, due to spin orbit coupling the singlet and triplet are mixed. It is the singlet component which gives the non-vanishing generalized oscillator strength and that is the curve shown in Fig. 5. The resonant energy transfer does not involve any change in multiplicity because only the singlet is active. Since the investigation is still in progress, the calculated cross sections shown in the table of Fig. 5 are still to some extent tentative.

The results described above were obtained while Winifred Huo was supported in part (20%) on our ERDA supported program from July 1 1975 to December 31, 1975. She is now supported by a Petroleum Research Fund (American Chemical Society) Grant (since January 1, 1976). The investigation is continuing under those auspices.

### 3. RESEARCH TO BE COMPLETED IN PRESENT CONTRACT PERIOD

Exploration of limiting kinetic energies for the transition  $E^3 \Sigma_g^+ \leftarrow X^1 \Sigma_g^+$  in  $N_2$  showed that the lens system between monochromator and collision cell must be revised for stable, low kinetic energy, operation. Revision of this lens system will be combined with modification of the collision cell (Section 2.2) to shorten the path length of electrons through the scattering cell. So as to avoid interference with operations while the singlet-triplet cross sections are completed (Section 2.5) a completely new unit, including electrostatic lenses, will be designed and constructed. This unit will be retained in standby condition until all experiments using the present cell have been com-



pleted. It is believed that the design and construction will be completed by July 1, 1976. If not, the project will be continued into the next contract period. The search for singlet-triplet transitions described in Section 2.4 will be deferred until this new cell and lens are installed. This probably means continuation into the next contract period.

The cross section study of Section 2.5 will be completed before July 1, 1976. Except for a few measurements at 300 eV, it is nearly complete now.

#### 4. STATUS OF RESEARCH SUPPORTED BY AFOSR AND NSF

A new electron spectrometer has been developed on a program supported with a grant from the Air Force Office of Scientific Research. This grant terminated on December 31, 1974 and was not extended. We did not have enough notice to obtain a replacement grant by January 1, 1975. However, a grant from the National Science Foundation was received for two years effective May 1, 1975. This enables the experimental part of the program to go forward with two persons, E. N. Lassette, Principal Investigator (35%) and Michael A. Dillon, Co-Principal Investigator (100%). This research involves the study of ionization continua using a newly developed spectrometer and fast coincidence techniques. There is no overlap or conflict with the program outlined in previous sections of the proposal, but it is believed that the results are of considerable interest in several areas of Radiological Physics. This spectrometer, with fast coincidence capability, is

believed to be the only operational instrument of its type in the United States and the most advanced design in existence anywhere.

The above grant from the National Science Foundation provides for Dr. Michael A. Dillon, who was supported by the AFOSR project before its termination. Dr. Winifred M. Huo was also supported by the AFOSR Grant before its termination on December 31, 1974. During all of 1975, Dr. Huo was supported mostly by Carnegie-Mellon University endowment funds except for 10% of her time on the present contract (she obtained equation 1 of Section 2.6 and tested it numerically during this time) and 10% on another project. To obtain further support for her, a proposal was submitted to the Petroleum Research Fund of the American Chemical Society (ACS). This grant was approved effective September 1, 1976, but we received permission to make an early beginning, January 1, 1976. The grant (E. N. Lassettre - Principal Investigator) pays  $2/3$  of Dr. Huo's salary. Carnegie-Mellon University pays the remainder. In view of the University's continued (perpetual?) financial stringency, a proposal was made to the National Science Foundation for the support of a theoretical program designed primarily to support the research of Dr. Huo and one post-doctoral fellow to be directed by her. A small fraction of the time of E. N. Lassettre would also be involved. A backup and somewhat modified, version of this proposal was submitted to the Physical Division of ERDA. Financial and other details are given in an accompanying renewal proposal.

All publications sponsored by ERDA since the beginning of the project are listed. Those sponsored by AFOSR over the same period are also listed. Those papers either submitted or published since the last proposal are marked with an asterisk.

## 5.1 Supported by ERDA

## 5.1.1 Published

- 1) Skerbele, A. and E. N. Lassettre, "Generalized Oscillator Strengths for the  $6^1S_0 \rightarrow 6^1P_1$  Transition in Mercury," Journal of Chemical Physics 52 (5), 2708-2711 (1970).
- 2) Skerbele, A. and E. N. Lassettre, "Absolute Electron Collision Cross Sections for Two Forbidden Transitions in Nitrogen at Kinetic Energies of 300-500 eV," Journal of Chemical Physics 53 (10), 3806 (1970).
- 3) Lassettre, E. N., "Further Selection Rules in Excitation by Electron Impact at Small Momentum Changes," Journal of Chemical Physics 53 (10), 3801 (1970).
- 4) Lassettre, E. N. and A. Skerbele, "Absolute Generalized Oscillator Strengths for Four Electronic Transitions in Carbon Monoxide," Journal of Chemical Physics 54, 1597-1607 (1971).
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- 6) Skerbele, A. and E. N. Lassettre, "Absolute Generalized Oscillator Strengths for Three Transitions in the Mercury Spectrum," Journal of Chemical Physics 56, 845-850 (1972).
- 7) Lassettre, E. N., "Power Series Expansion of Collision Amplitudes. Electrostatic Potentials," Journal of Chemical Physics 57, 4357-4369 (1972).
- 8) Harshbarger, W. R. and E. N. Lassettre, "Electron Impact Spectra of  $CH_4$  and  $CF_4$ ," Journal of Chemical Physics 58, 1505 (1973).

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- 12) Skerbele, A. and E. N. Lassettre, "Generalized Oscillator Strengths for the Excitation of Heavy Atoms:  $6^1S_0 \rightarrow 6^1P_1$ ,  $6^1S_0 \rightarrow 7^1S_0$  and  $6^1S_0 \rightarrow 7^1P_1$  Transitions in Mercury," Journal of Chemical Physics 58, 2887 (1973).
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- 14) Lassettre, E. N. and A. Skerbele, "Generalized Oscillator Strengths for 7.4 eV Excitation of  $H_2O$  at 300, 400 and 500 eV Kinetic Energy. Singlet-Triplet Energy Differences," Journal of Chemical Physics 60, 2464 (1974).
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#### 6. PERSONNEL

Personnel were Dr. E. N. Lassettre (65% for 12 months), Dr. Kirby N. Klump (100% for 12 months), and Dr. Winifred M. Huo (20% for 6 months).

#### 7. NEW APPARATUS

A new pressure gauge, a capacitance manometer, has been purchased and installed for the precise measurement of pressure in the collision cell. The purchase price of this instrument (\$2,793.00) has been shared equally between ERDA and Carnegie-Mellon University.