Chapter 3

Calculation of scattering cross sections

As described in chapter I, the present experiment measures the total electron scattering cross sections from the attenuation of intensity of different photoelectron peaks by the target gas. Two different analytical procedures have been used depending upon whether the source and the target gases are same or different. Both these methods developed previously have been discussed briefly by Kumar et al (1987).

Total electron scattering cross sections for Carbon dioxide \((CO_2)\), Carbon monoxide \((CO)\) and Nitrous oxide \((N_2O)\) were calculated from the photoelectron peak-attenuation data using these methods. The methods are being described below.
3.1 When the source and the target gas are different

The following method is used when the source gas is different from the target gas. In this class of experiment, the source gas is introduced into the ionization chamber at a partial pressure \( P_s \). \( P_s \) has a low and constant value throughout the experiment. The interaction of photons with the source gas produces photoionization and electrons are liberated. The target gas is then introduced into the same region at partial pressures \( P_1, P_2, P_3, \ldots \) etc, which results in the attenuation of the number of electrons reaching the detector. This attenuation of electron intensity is given by the Beer-Lambert law. According to this law, the electron intensity, \( I_e \), detected after passing through a path length \( x \) in a gas with number density \( n \) and scattering cross section \( \sigma_{sc} \), is related to the initial intensity \( I_0 \) as

\[
I_e = I_0 e^{-n_0 n x}
\]

The number density of a gas at pressure \( P \), at room temperature is

\[
n = \frac{n_0 P}{760}
\]

where \( n_0 \) is the Loschmidt’s number, \( 2.688 \times 10^{19}/cm^3 \). Putting (3.2) into (3.1) gives

\[
I_e = I_0 e^{-\frac{n_0 P}{760} \sigma_{sc} x}
\]

When \( I_{e1}, I_{e2}, I_{e3}, \ldots \) etc., are the electron intensities at the respective target gas pressures \( P_1, P_2, P_3, \ldots \) etc., and when \( I_{e01}, I_{e02}, I_{e03}, \ldots \) etc., are the respective initial electron intensities, then

\[
I_{e1} = I_{e01} e^{-\frac{n_0}{760} (P_1 \sigma_{sc}^1 + P_1 \sigma_{sc}^1) x}
\]

\[
I_{e2} = I_{e02} e^{-\frac{n_0}{760} (P_2 \sigma_{sc}^2 + P_2 \sigma_{sc}^2) x}
\]

and so on. \( \sigma_{sc}^1 \) and \( \sigma_{sc}^2 \) in the above equations are the scattering cross sections of the source and target gases respectively. Ratio of (3.4) and (3.5) gives

\[
\frac{I_{e1}}{I_{e2}} = \frac{I_{e01}}{I_{e02}} e^{-\frac{n_0}{760} (P_1 - P_2) \sigma_{sc} x}
\]
Figure 3.1: Schematic diagram showing some parts of photon and electron path lengths in the experiment

The number of photoelectrons generated, \( I_{e0} \), depends upon the ionizing photon beam intensity, \( I_\lambda \), the number of gas molecules, \( n \), the ionization cross section of the source gas, \( \sigma_{ion} \), and \( \Delta l \), the length over which ionization takes place. Hence,

\[
I_{e0} = n I_\lambda \sigma_{ion} \Delta l
\]  
(3.7)

Since, the source gas pressure remains constant throughout the experiment,

\[
I_{e01} = n I_{\lambda 1} \sigma_{ion} \Delta l
\]  
(3.8)

and

\[
I_{e02} = n I_{\lambda 2} \sigma_{ion} \Delta l
\]  
(3.9)

or

\[
\frac{I_{e01}}{I_{e02}} = \frac{I_{\lambda 1}}{I_{\lambda 2}}
\]  
(3.10)
The VUV photon beam reaches the ionization region after traveling a length \( l \) from the beam splitter. The relation between the light intensity at the beam splitter, \( I_{0} \), to that in the ionizing region, \( I_{\lambda} \), is also given by the Beer-Lambert law. Thus,

\[
I_{\lambda} = I_{0} e^{-\sigma_{ab} l}
\]

(3.11)

where \( \sigma_{ab} \) is the photoabsorption cross section. Putting (3.2) into (3.11) gives

\[
I_{\lambda} = I_{0} e^{-\sigma_{ab} l}
\]

(3.12)

where \( P \) is the corresponding gas pressure. As can be seen from figure 3.1, the path length \( l \) in the experiment is divided into two parts, \( l_{1} \) and \( l_{2} \). The path \( l_{2} \) lies within the ionization chamber and \( l_{1} \) outside it. The geometry of the apparatus makes the gas pressure outside the ionization chamber a fraction of that inside it. The variation of pressure outside the ionization chamber, \( P'' \), with respect to that inside it, \( P' \), is linear over a wide range of pressures and the ratio of pressures, in the range of \( 10^{-3} - 5 \times 10^{-2} \) Torr, has been found to be constant.

\[
a = \frac{P''}{P}
\]

(3.13)

\[
a = 0.124
\]

(3.14)

Thus, in the presence of both, the source and the target gases, equation (3.12) gives

\[
I_{\lambda_{1}} = I_{0} e^{-\sigma_{ab} l_{1}} \left[ P'_{s} \sigma_{ab l_{1}} + P'_{t} \sigma_{ab l_{1}} + P'_{t_{2}} \sigma_{ab l_{1}} \right]
\]

(3.15)

and similarly

\[
I_{\lambda_{2}} = I_{0} e^{-\sigma_{ab} l_{2}} \left[ P'_{s} \sigma_{ab l_{2}} + P'_{t} \sigma_{ab l_{2}} + P'_{t_{2}} \sigma_{ab l_{2}} \right]
\]

(3.16)

where \( \sigma_{ab} \) and \( \sigma_{ab} \) are the absorption cross sections for the source gas and the target gas respectively. The present quantities, \( P'_{s} \), \( P'_{t_{1}} \), and \( P'_{t_{2}} \) are pressures outside the ionization chamber corresponding to \( P'_{s} \), \( P'_{t_{1}} \), and \( P'_{t_{2}} \) respectively, and the relation between them is given by (3.13), i.e.

\[
P'_{s} = a P_{s}
\]

(3.17)

\[
P'_{t_{1}} = a P_{t_{1}}
\]

(3.18)

\[
P'_{t_{2}} = a P_{t_{2}}
\]

(3.19)
Since, $n_0 \times \sigma_{ab} = k_{ab}^0$, the photoabsorption coefficient for the target gas, expression becomes

$$\frac{I_{\lambda_1}}{I_{\lambda_2}} = \frac{I_{\lambda_{10}}}{I_{\lambda_{20}}} e^{-\frac{x_{10}}{\lambda_0} (P_{11} - P_{12}) (n_1 + n_2)} \times e^{-\frac{x_{20}}{\lambda_0} (P_{21} - P_{22}) \sigma_{a1}^r}$$  \(3.24\)

putting (3.24) into (3.10) gives

$$\frac{I_{\lambda_{10}}}{I_{\lambda_{20}}} = \frac{I_{\lambda_{11}}}{I_{\lambda_{21}}} e^{-\frac{x_{11}}{\lambda_0} (P_{11} - P_{12}) (n_1 + n_2)}$$  \(3.25\)

putting (3.25) into (3.6) gives

$$\frac{I_{e_1}}{I_{e_2}} = \frac{I_{\lambda_{10}}}{I_{\lambda_{20}}} e^{-\frac{x_{11}}{\lambda_0} (P_{11} - P_{12}) (n_1 + n_2)} \times e^{-\frac{x_{20}}{\lambda_0} (P_{21} - P_{22}) \sigma_{a1}^r}$$  \(3.26\)

or

$$\frac{I_{e_1}}{I_{e_2}} = \frac{I_{\lambda_{10}}}{I_{\lambda_{20}}} e^{-\frac{(P_{11} - P_{12})}{\lambda_0} [\sigma_{a1}^r (n_1 + n_2) + \sigma_{a1}^r \sigma_{a1}^r]}$$  \(3.27\)

or

$$\frac{I_{e_1}}{I_{e_2}} = \frac{I_{\lambda_{10}}}{I_{\lambda_{20}}} e^{-\frac{(P_{11} - P_{12})}{\lambda_0} [\sigma_{a1}^r (n_1 + n_2) + \sigma_{a1}^r \sigma_{a1}^r]}$$  \(3.28\)

or

$$\ln \left[ \frac{I_{\lambda_{10}}}{I_{\lambda_{10}}} \frac{I_{\lambda_{20}}}{I_{\lambda_{20}}} \right] = \frac{(P_{11} - P_{12})}{\lambda_0} \left[ \sigma_{a1}^r (n_1 + n_2) + \sigma_{a1}^r \sigma_{a1}^r \right]$$  \(3.29\)

It needs to be pointed out that, though, the absolute values of $I_{\lambda_{10}}$ and $I_{\lambda_{20}}$ cannot be found out in the present experiment, the ratio $\frac{I_{\lambda_{10}}}{I_{\lambda_{20}}}$ can be found out from the beam splitter arrangement. In the above relation (equation 3.29), quantities $I_{e_1}$, $I_{e_2}$, $P_{11}$, $P_{12}$ and the ratio $\frac{I_{\lambda_{10}}}{I_{\lambda_{20}}}$, are the observables and $x$, $a$, $l_1$ and $l_2$ are the constants of the experiment known from the geometry of the apparatus. While $n_0$ is the Loschmidt's
number, the value of \( k_{ab}' \) is taken from the literature. Values of \( k_{ab}' \) used in the calculations, for different wavelengths for the three target gases are given in table 3.1. Putting all these quantities in (3.29) yields the total scattering cross section, \( \sigma_{t'}^{f} \), for the target gas.

Table 3.1: Values of photoabsorption co-efficients for the target gases at three wavelengths in VUV region.

<table>
<thead>
<tr>
<th>Target gas</th>
<th>VUV wavelength</th>
<th>Absorption co-efficient</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Å</td>
<td>cm(^{-1})</td>
<td></td>
</tr>
<tr>
<td>Carbon</td>
<td>584</td>
<td>966.9</td>
<td>Samson &amp; Yin (1989)</td>
</tr>
<tr>
<td>dioxide</td>
<td>736</td>
<td>624.7</td>
<td>&quot;</td>
</tr>
<tr>
<td></td>
<td>744</td>
<td>375.0</td>
<td>&quot;</td>
</tr>
<tr>
<td>Carbon</td>
<td>584</td>
<td>558.7</td>
<td>&quot;</td>
</tr>
<tr>
<td>monoxide</td>
<td>736</td>
<td>615.0</td>
<td>&quot;</td>
</tr>
<tr>
<td></td>
<td>744</td>
<td>510.4</td>
<td>&quot;</td>
</tr>
<tr>
<td>Nitrous</td>
<td>584</td>
<td>986.8</td>
<td>&quot;</td>
</tr>
<tr>
<td>oxide</td>
<td>736</td>
<td>1088.4</td>
<td>&quot;</td>
</tr>
<tr>
<td></td>
<td>744</td>
<td>1136.2</td>
<td>&quot;</td>
</tr>
</tbody>
</table>

\( k_{ab}' (a_0 + l_2) \) on the right hand side in (3.29) is a correction term. Equation 3.29 being an equation of a straight line \( y = mx + c \), where \( c = 0 \) plot of \( \ln \left[ \frac{l_1}{l_2} \right] \) vs \( \left( p_1 - p_2 \right) \) yields a straight line whose slope leads to the value of the total scattering cross section \( \sigma_{t'}^{f} \).

3.2 When source and target gas are the same

In this second case, the source gas is same as the target gas. In this class of experiments, photoelectrons generated by the gas under study are scattered by itself. The photoelectron production rate, unlike in the case of experiment discussed in the previous section, changes throughout the experiment as the pressure of the source/target gas is increased. The number of photoelectrons detected is a resultant of the two competing...
phenomena, viz, production and scattering of electrons. While the photoelectron production rate is proportional to the number density of gas molecules (or pressure, P), scattering is related to the inverse of exponential of pressure, P. Thus, the actual detected intensity is

\[ I \propto P^{-n} \]  \hspace{1cm} (3.30)

where 'n' is a parameter containing the scattering cross section.

The starting point in the analysis of the method of calculation of total scattering cross section from the data collected by this class of experiment is also the Beer-Lambert law, of the form of (3.3), i.e.:

\[ I = I_0 e^{-\frac{n_0}{n_1} \sigma_n} \]  \hspace{1cm} (3.31)

All the quantities in the above expression mean the same as in the previous section. As the source gas and the target gas are the same, 's' and 't' in the superscripts and subscripts become redundant and (3.4) and (3.5) assume the form

\[ I_{t1} = I_{e01} e^{-\frac{n_0}{n_1} \sigma_n} \]  \hspace{1cm} (3.32)

and

\[ I_{t2} = I_{e02} e^{-\frac{n_0}{n_1} \sigma_n} \]  \hspace{1cm} (3.33)

Thus,

\[ \frac{I_{t1}}{I_{t2}} = \frac{I_{e01}}{I_{e02}} e^{-\frac{n_0}{n_1} (P_1 - P_2) \sigma_n} \]  \hspace{1cm} (3.34)

The initial electron intensities, 'I_{e01}' and 'I_{e02}', are given, again, by (3.7), i.e.

\[ I_{e0} = n_1 \sigma_{n1} \Delta l \]  \hspace{1cm} (3.35)

But since the gas pressure changes in this case, (3.8) and (3.9) become

\[ I_{e01} = n_1 I_{s1} \sigma_{n1} \Delta l \]  \hspace{1cm} (3.36)

and

\[ I_{e02} = n_2 I_{s2} \sigma_{n2} \Delta l \]  \hspace{1cm} (3.37)

Their ratio, thus, becomes

\[ \frac{I_{e01}}{I_{e02}} = \frac{n_1 I_{s1}}{n_2 I_{s2}} \]  \hspace{1cm} (3.38)
Since, here

\[ n_1 = \frac{n_0 P_1}{l_60} \]  \hspace{0.5cm} (3.39)

and

\[ n_2 = \frac{n_0 P_2}{l_60} \]  \hspace{0.5cm} (3.40)

(3.38) becomes

\[ \frac{I_{1\text{in}}}{I_{2\text{in}}} = \frac{P_1}{P_2} \frac{I_{1\text{in}}}{I_{2\text{in}}} \]  \hspace{0.5cm} (3.41)

Drawing a parallel from (3.15) and (3.16) we have

\[ I_{\lambda_1} = I_{\lambda_01} e^{-\frac{n_0}{l_60} [p_{1\text{in}} l_1 + p_{2\text{out}} l_2]} \]  \hspace{0.5cm} (3.42)

and

\[ I_{\lambda_2} = I_{\lambda_02} e^{-\frac{n_0}{l_60} [p_{1\text{in}} l_1 + p_{2\text{out}} l_2]} \]  \hspace{0.5cm} (3.43)

Here

\[ P'_1 = a P_1 \]  \hspace{0.5cm} (3.44)

\[ P'_2 = a P_2 \]  \hspace{0.5cm} (3.45)

Putting (3.44) and (3.45) in (3.42) and (3.43) respectively, gives

\[ I_{\lambda_1} = I_{\lambda_01} e^{-\frac{n_0}{l_60} [p'_1 l_1 + p'_2 l_2]} \]  \hspace{0.5cm} (3.46)

and

\[ I_{\lambda_2} = I_{\lambda_02} e^{-\frac{n_0}{l_60} [p'_1 l_1 + p'_2 l_2]} \]  \hspace{0.5cm} (3.47)

Putting (3.46) and (3.47) into (3.41) gives

\[ \frac{I_{1\text{in}}}{I_{2\text{in}}} = \frac{P_1}{P_2} \frac{I_{1\text{in}}}{I_{2\text{in}}} e^{-\frac{n_0}{l_60} [p'_1 l_1 + p'_2 l_2]} \]  \hspace{0.5cm} (3.48)

Putting (3.48) into (3.34) gives

\[ \frac{I_{1\text{in}}}{I_{2\text{in}}} = \frac{P_1 I_{\lambda_01}}{P_2 I_{\lambda_02}} e^{-\frac{n_0}{l_60} [p'_1 l_1 + p'_2 l_2]} e^{-\frac{n_0}{l_60} [p_{1\text{in}} l_1 + p_{2\text{out}} l_2]} \]  \hspace{0.5cm} (3.49)

or

\[ \frac{I_{1\text{in}}}{I_{2\text{in}}} = \frac{P_1 I_{\lambda_01}}{P_2 I_{\lambda_02}} e^{-\frac{n_0}{l_60} [p_{1\text{in}} l_1 + p_{2\text{out}} l_2 + n_0 \sigma_{ab}]} \]  \hspace{0.5cm} (3.50)

Since,

\[ n_{ab} \sigma_{ab} = \hbar_{ab} \]  \hspace{0.5cm} (3.51)
where \( k_{ab} \) is the photoabsorption co-efficient. The expression becomes

\[
\frac{I_{t1}}{I_{t2}} = \frac{P_1 I_{\lambda 1}}{P_2 I_{\lambda 2}} e^{-\frac{(n_1 - n_2)}{760} \left[ n_0 \sigma_{e} + \frac{k_{ab}}{n_1 n_2} (n_1 + n_2) \right]} 
\]  

or

\[
L_n \left[ \frac{I_{t1} P_1 I_{\lambda 1}}{I_{t2} P_2 I_{\lambda 2}} \right] = \frac{P_1 - P_2}{760} \left[ n_0 \sigma_{e} + k_{ab} (n_1 + n_2) \right] 
\]

The above expression gives the total electron scattering cross section when the target and the source gases are the same.

Similar to the previous case, a plot of \( L_n \left[ \frac{I_{t1} P_1 I_{\lambda 1}}{I_{t2} P_2 I_{\lambda 2}} \right] \) vs \( (P_1 - P_2) \) is a straight line whose slope gives the total scattering cross section, \( \sigma_e \).

The different quantities used in the derivation of total scattering cross section have been summarized in table 3.2. The values of the constants could be found from the geometry of the experimental system used in the present work. These are:

\[
x = 2.37 \text{ cms} \quad a = 0.124
\]
\[
I_1 = 30 \text{ cms} \quad I_2 = 2.58 \text{ cms}
\]

Table 3.2: Summary of different quantities used in the derivation of total scattering cross section.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( P_s' )</td>
<td>Source gas pressure inside the ionization chamber</td>
</tr>
<tr>
<td>( P_s'' )</td>
<td>Source gas pressure outside the ionization chamber</td>
</tr>
<tr>
<td>( P_{t1}, P_{t2}, \ldots )</td>
<td>Target gas pressures inside the ionization chamber</td>
</tr>
<tr>
<td>( P_{t1}', P_{t2}', \ldots )</td>
<td>Target gas pressures outside the ionization chamber</td>
</tr>
<tr>
<td>( \sigma_{e}' )</td>
<td>Source gas total scattering cross section</td>
</tr>
<tr>
<td>( \sigma_{t}' )</td>
<td>Target gas total scattering cross section</td>
</tr>
<tr>
<td>( \sigma_{ab}' )</td>
<td>Source gas photoabsorption cross section</td>
</tr>
<tr>
<td>( \sigma_{tab}' )</td>
<td>Target gas photoabsorption cross section</td>
</tr>
<tr>
<td>( \sigma_{eim} )</td>
<td>Source gas photodetachment cross section</td>
</tr>
<tr>
<td>( k_{ab} )</td>
<td>Source gas photoabsorption co-efficient</td>
</tr>
</tbody>
</table>