Ion mobility in Xe-CO2 mixtures: recent results


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Chronogram

Feb | Mar | April | May | June

Xe-C2H6 mixture  2/2/17  8/3/17

Ar-N2 mixture  16/3/17  30/4/17

Xe-CH4 mixture  1/5/17  15/6/17

Design of a chamber to measure mobility of negative ions within a Collaboration with JINR  15/4/17
1 Basic Concepts

2 Experimental Setup and Working Principle

3 Ion Identification Process

4 Experimental results in:
   a Xe, CO₂
   b Xe-CO₂
Let us consider a group of ions moving in a gaseous medium under the influence of a uniform electric field...

**Drift velocity**

\[ v_d = KE \]

- \( E \)- Electric Field
- \( K \)- Ion Mobility

**Reduced Mobility**

\[ K_0 = \frac{KN}{N_0} \]

- \( N \)- Gas number density
- \( N_0 \)- Loschmidt Number

**Langevin Limit**

\[ K_0 = 13.88 \left( \frac{1}{\alpha \mu} \right)^{\frac{1}{2}} \]

- \( \mu \)- reduced mass
- \( \alpha \)- neutral polarizability

**Blanc’s Law**

\[ \frac{1}{K_{0\text{mix}}} = \frac{f_1}{K_{0g1}} + \frac{f_2}{K_{0g2}} \]

- \( f_1, f_2 \)- molar fraction of gas 1, 2
- \( K_{0g1}, K_{0g2} \)- ion mobility in the gas 1 and 2
Experimental Setup and Working Principle

- Xenon UV flash lamp: 10Hz, <500ns
- G1
- G2= Frisch Grid

Charge Pre-amplifier

Digital Oscilloscope

GEM

CsI

(Neves, Conde and Távora, 2007)
Experimental Setup and Working Principle

- Subtract the background to the signal
- Identify possible peaks
- Fit Gaussian curves to the peaks obtained

Peaks centroids

\[ v_d = \frac{x_{\text{drift}}}{t_{\text{drift}}} \]
\[ K = \frac{v_d}{E} \]

\[ K_{01} = 1.57 \text{ cm}^2\text{V}^{-1}\text{s}^{-1} \quad (\text{Ar}^+) \]
\[ K_{02} = 1.92 \text{ cm}^2\text{V}^{-1}\text{s}^{-1} \quad (\text{Ar}_2^+) \]
Ion Identification Process

Identification of candidate ions
- GEM Voltage
- Possible Reactions
  - Cross Section
  - Reaction Rates

Selection of Candidate ions

Calculation of expected mobility
- Langevin Limit (formula)
- Blanc’s law (mixtures)

Comparison with experimental results

Theoretical Values = Experimental Values

Match?
Ion Mobility Measurement at LIP Coimbra

**Ionization**

\[ \text{Xe} + e^- \rightarrow \text{Xe}^+ + 2e^- \]

**Secondary Reactions**

\[ \text{Xe}^+ + 2\text{Xe} \rightarrow \text{Xe}_2^+ + \text{Xe} \]
\[ \text{Xe}^+ + \text{Xe} \rightarrow \text{Xe} + \text{Xe}^+ \]

Above 12.1 eV

**Experimental Results: Xe**

\[ K_{01} = 0.58 \text{ cm}^2\text{V}^{-1}\text{s}^{-1} (\text{Xe}^+ ) \]
\[ K_{02} = 0.64 \text{ cm}^2\text{V}^{-1}\text{s}^{-1} (\text{Xe}_2^+ ) \]

P.N.B. Neves, 2011, IEEE

E/N=20 Td
7,992 Torr
\[ V_{\text{GEM}} = 16 \text{ V} \]
**Experimental Results: CO₂**

**Ionization**

\[ \text{CO}_2 + e^- \rightarrow \text{CO}_2^+ + 2e^- \]  
Above 13.8 eV

\[ \text{CO}_2 + e^- \rightarrow \text{CO}_2^+ + 2e^- \]  
\[ \rightarrow \text{CO}^+ + \frac{1}{2}\text{O}_2 + 2e^- \]  
\[ \rightarrow \text{O}^+ + \text{CO} + 2e^- \]  
Above 19.5 eV

**Appearance Energies**

- \( \text{CO}_2^+ \): 13.8 eV
- \( \text{CO}^+ \): 19.5 eV
- \( \text{O}^+ \): 19.1 eV

**Secondary Reactions**

- \( \text{CO}_2^+ + \text{CO}_2 \rightarrow \text{CO}_2 + \text{CO}_2^+ \)
- \( \text{CO}^+ + \text{CO}_2 \rightarrow \text{CO}_2^+ + \text{CO} \)
- \( \text{O}^+ + \text{CO}_2 \rightarrow \text{O}_2^+ + \text{CO} \)

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P.M.C.C. Encarnação, 2015, JINST
Experimental Results: CO$_2$

$K_{01} \sim 1.17 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$

CO$_2^+$

Good agreement with earlier reported works:

1. W. T. Huntress et al.: 1.23 cm$^2$V$^{-1}$s$^{-1}$
2. G. Schultz et al.: 1.09 cm$^2$V$^{-1}$s$^{-1}$

Langevin Formula

1.82 cm$^2$V$^{-1}$s$^{-1}$

$\neq$

Extrapolated Value
$(E/N \rightarrow 0)$

1.17 cm$^2$V$^{-1}$s$^{-1}$

Charge Transfer Process

CO$_2^+$ + CO$_2$ $\rightarrow$ CO$_2$ + CO$_2^+$

CO$_2^+$ + CO$_2$ + M $\rightarrow$ CO$_2$.CO$_2^+$ + M

Graph:

- Experimental results
- G.schultz [CO2+]
- W. T. Huntress [CO2+]
- P.A. Coxon et al [CO2+(CO2)n]
Experimental Results: Xe-CO$_2$

- **15% Xe**
  - Xe$^+$

- **25% Xe**
  - Xe$^+/\text{Xe}_2^+$

- **50% Xe**
  - Xe$_2^+$

- **95% Xe**
  - Xe$_2^+$

**Experimental Conditions:**
- E/N = 15 Td
- P = 8 Torr
- VGEM = 25 V

Ion Mobility Measurement at LIP Coimbra
Experimental Results: Xe-CO$_2$

**Direct Ionization**

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Cross Section (20 eV)</th>
<th>Final Ion</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO$_2$ + e $\rightarrow$ CO$_2^+$ + 2e</td>
<td>0.452</td>
<td>CO$_2^+$</td>
</tr>
<tr>
<td>Xe + e $\rightarrow$ Xe$^+$ + 2e</td>
<td>2.43</td>
<td>Xe$^+$</td>
</tr>
</tbody>
</table>

**Xe$^+$** predominant primary ion down to **15%** of Xe.

**Secondary Reactions**

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Rate Constant cm$^3$.s$^{-1}$ or cm$^6$.s$^{-1}$</th>
<th>Final Ion</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO$_2^+$ + Xe $\rightarrow$ CO$_2$ + Xe$^+$</td>
<td>6E-10</td>
<td>Xe$^+$</td>
</tr>
<tr>
<td>Xe$^+$ + Xe $\rightarrow$ Xe + Xe$^+$</td>
<td>2.5E-10</td>
<td>Xe$^+$</td>
</tr>
<tr>
<td>Xe$^+$ + 2Xe $\rightarrow$ Xe$_2^+$ + Xe</td>
<td>2E-31</td>
<td>Xe$_2^+$</td>
</tr>
<tr>
<td>CO$_2^+$ + CO$_2$ + M $\rightarrow$ CO$_2$.CO$_2^+$ + M</td>
<td>2.1E-28</td>
<td>CO$_2$.CO$_2^+$</td>
</tr>
<tr>
<td>CO$_2^+$ + CO$_2$ $\rightarrow$ CO$_2$ + CO$_2^+$</td>
<td>3.7E-10</td>
<td>CO$_2^+$</td>
</tr>
</tbody>
</table>

**E/N = 20 Td**

P = 8 Torr (95% Xe 5% CO$_2$)

VGEM = 25 V
Reactions Paths

\[ K_{01} \sim 0.99 \text{ cm}^2\text{V}^{-1}\text{s}^{-1} \]

\[ K_{01} \sim 0.93 \text{ cm}^2\text{V}^{-1}\text{s}^{-1} \]

\[ K_{01} \sim 0.82 \text{ cm}^2\text{V}^{-1}\text{s}^{-1} \]
Experimental Results: Xe-CO₂

P = 8 Torr
V_GEM = 25V
E/N = 15 Td

Ion Mobility Measurement at LIP Coimbra

Experimental Results: Xe-CO₂

P = 8 Torr
V_GEM = 25V
E/N = 15 Td

Ion Mobility Measurement at LIP Coimbra

Experimental Results: Xe-CO₂

P = 8 Torr
V_GEM = 25V
E/N = 15 Td

Ion Mobility Measurement at LIP Coimbra
Present Status and Future Work

• Pursuit the investigation of the mobility of ions in different gas mixtures of practical use (if you have any suggestions feel free to contact us).
  • In the scope of the RD51 common project submitted with GSI (Germany), Uludag Univ. (Turkey) and VECC (India).

\( \text{Ne-N}_2 \) (Published)
\( \text{Ne-CO}_2-N_2 \) (Presented in IEEE NSS Conference 2016 - Strasbourg)
\( \text{Xe-CO}_2 \) (Finished – Paper Submitted to JINST)
\( \text{Xe-C}_2\text{H}_6 \) (Ongoing with Preliminary Results)
\( \text{Ar-N}_2 \)
\( \text{Ar-CF}_4 \) and \( \text{Ar-CF}_4\)-IsoButane

• Rate constant influence
• Study lighter ions (\( \text{H}_2 \))
• Water influence on the ion’s mobility
• (...)

• Optimization of the detector:
  • \textit{Variable Drift Distance}
    (Already designed ready to be implemented – done by P. Encarnação)
  • \textit{Measurement of the mobility of negative ions}
    (Just started the design of it within a Collaboration with JINR)
• A special thank to FCT-Fundação para a Ciência e Tecnologia for supporting this work through the National funds in the frame of the Project QREN n.4825, Rad for Life and to

• CERN/RD51 Collaboration – Common Projects - ‘Measurement and calculation of ion mobility of some gas mixtures of interest’. Participating institutions:

Thank you!
Mixing Langevin Limit with Blanc’s Law

**Langevin Limit**
To determine the mobility of an ion within a gas (not the parent).

\[ K_p = 13.88 \left( \frac{1}{\alpha \mu} \right)^{\frac{1}{2}} \]

\( \mu \) – reduced mass
\( \alpha \) – neutral polarizability

**Experimental Ion Mobility Values**
Mobility of an ion within his parent gas (if known).

**Theoretical Mobility Values**

**Blanc’s Law**
Used to calculate the mobility of an ion in a gas mixture.

\[ \frac{1}{K_{0\text{mix}}} = \frac{f_1}{K_{0g1}} + \frac{f_2}{K_{0g2}} \]

\( f_1, f_2 \) – molar fraction of gas 1 and 2

**Mobility of an ion in a mixture**
Candidate ions identification

**GEM Voltage**
- Maximum energy gained by electrons.
- Primary ions possible to be formed.

\[
\text{Rg (pure)} \\
\text{Rg} + \text{e} \rightarrow \text{Rg}^+ + 2\text{e}
\]

**Possible Reactions**
Ions formed through reactions of the primary ions with neutral atoms or molecules from the medium.

**Select Most Probable Ions**
Used to calculate the mobility of an ion in a gas mixture.

\[
\tau = \frac{1}{kN}
\]
- Identification the possible ions present.

**Reaction Time**
Used to calculate the variation of the concentration of a specific ion in a mixture.

\[
\frac{[\text{Rg}^+]}{[\text{Rg}^+]_0} = e^{-\frac{t}{\tau}} \\
\frac{[\text{X}^+]}{[\text{X}^+]_0} = 1 - \frac{[\text{Rg}^+]}{[\text{Rg}^+]_0}
\]
- Identification the possible ions present.

**Universal decay law**
Reactions Paths

\[ \text{Ne}^+ + \text{N}_2 \rightarrow \text{N}_2^+ + \text{Ne} \]

\[ \text{N}_2^+ + 2\text{N}_2 \rightarrow \text{N}_4^+ + \text{N}_2 \]

\[ \text{N}_2^+ + 2\text{N}_2 \rightarrow \text{N}_4^+ + \text{N}_2 \]

\[ \sim 35 \mu s \]
Ion mobility results comparison

![Graph showing ion mobility results comparison](image)