Calculation of TOF of molecule using TOFMS Technique

Report on Study Course

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Submitted to

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Content

Abstract

A TOFMS (time of flight mass spectrometer) is used to calculate Time of Flight of the ions. Here I have used a channeltron for the detection of time of start of ions and a MCP (Micro channel plate) for the detection of the time at which ions reach at the MCP. A C- program is used for the calculation of time of flight of Deuteron. By using ROOT a time-histogram is made for the data obtained by C-program.

Time of Flight mass Spectrometer

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1- Atomic Mass Spectrometer:

Atomic mass spectrometer is an instrument that produces ions and separates them according to their mass-to-charge ratios (m/z). It identifies a sample by measuring its molecular weight.
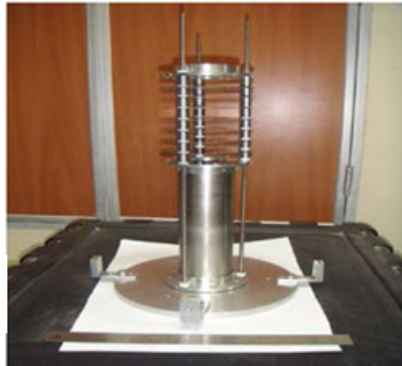
Components of an Atomic mass spectrometer:
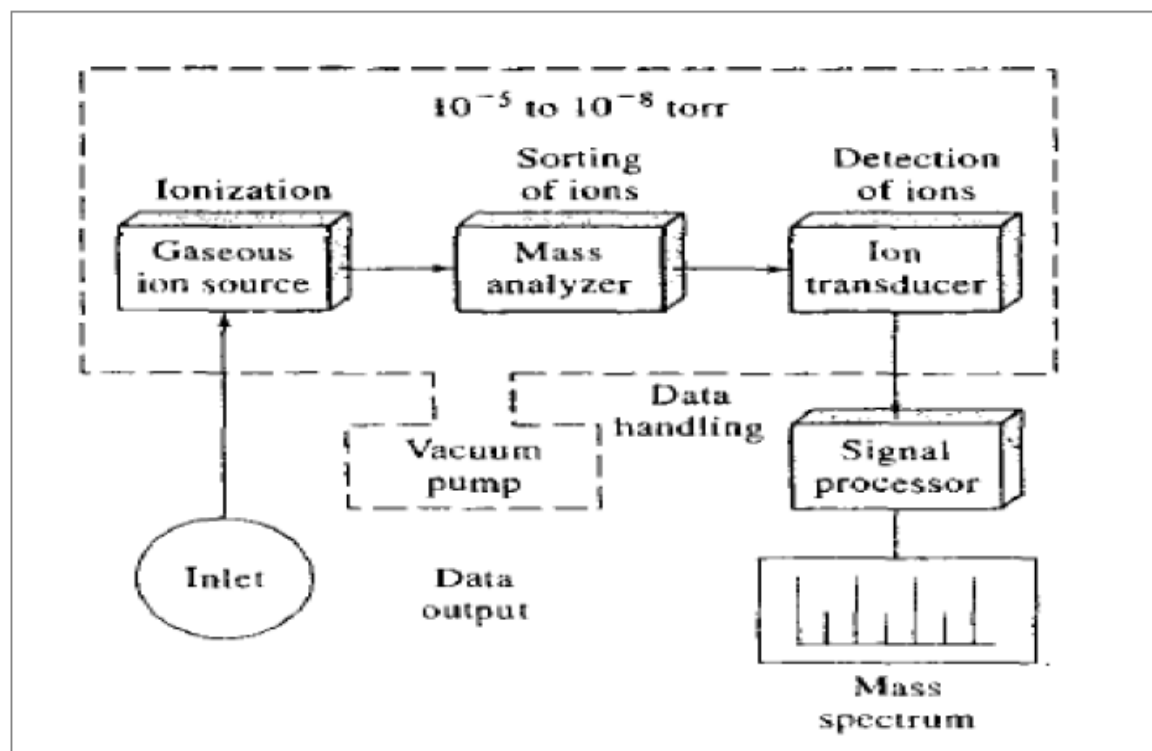
2- Principle of a TOF mass Analyzer:

It is one of the analytical technique in mass spectrometry. When sample molecules are ionized, an electrical field accelerates all of them to the same energy. The velocity of a molecule is given by

$$velocity = \sqrt{\frac{2 \times energy}{mass}}$$

The speed of an ion is depend on its mass. heavy ions having a lower velocity than light ones. The accelerated ions then enter into a field free (drift) region and we measure the time taken by the ions by the following formula.

$$Flight\_time = \frac{drift\_length}{velocity} = drift\_length \times \sqrt{\frac{mass}{2 \times energy}}$$

A start velocity is dependent upon their mass, measuring the flight time each ion takes to fly through the drift region is just proportional to the square root of their mass.

A detector at the end of the field-free region then records a signal as it is struck by each ion. The difference between the common start time of all ions and the detection time of an individual ion can then be used to calculate its mass to charge ratio (m/z).

3- Ion Reflectron in Time-of-Flight Mass Spectrometry:

Ions pass along the flight tube until they reach the reflectron. The reflectron then redirects the ions back along the same flight tube at a slightly different angle. Ions of a higher kinetic energy arrive at the reflectron earlier and penetrate deeper than ions of the same m/z but with lower kinetic energy.

Therefore, ions with the same m/z yet different energies will meet at the reflectron at different time.The addition of a reflectron also increases the length of the flight path, further enhancing resolution
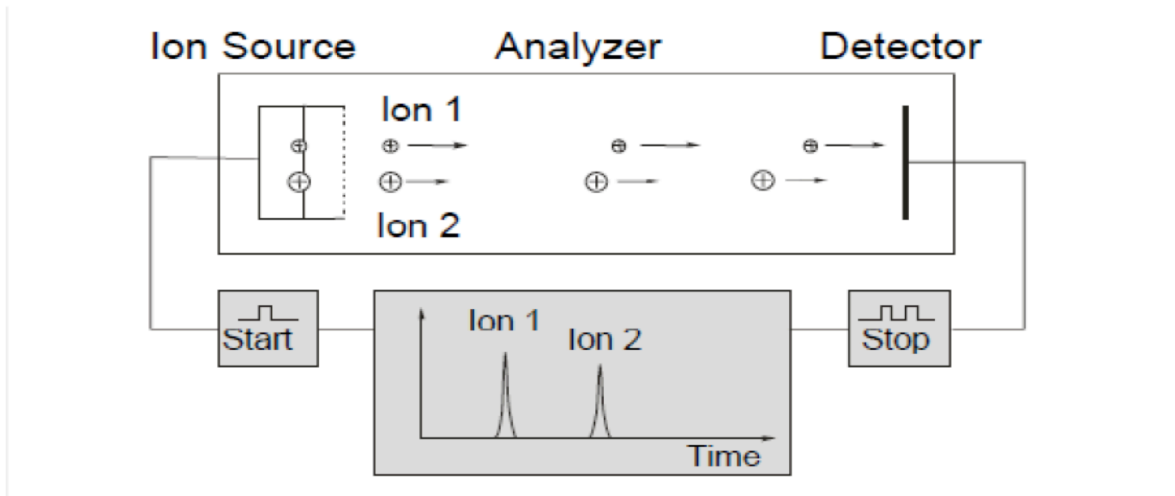
by allowing more time for separation of ions of differing m/z ratio, without unduly increasing the size of the instrument
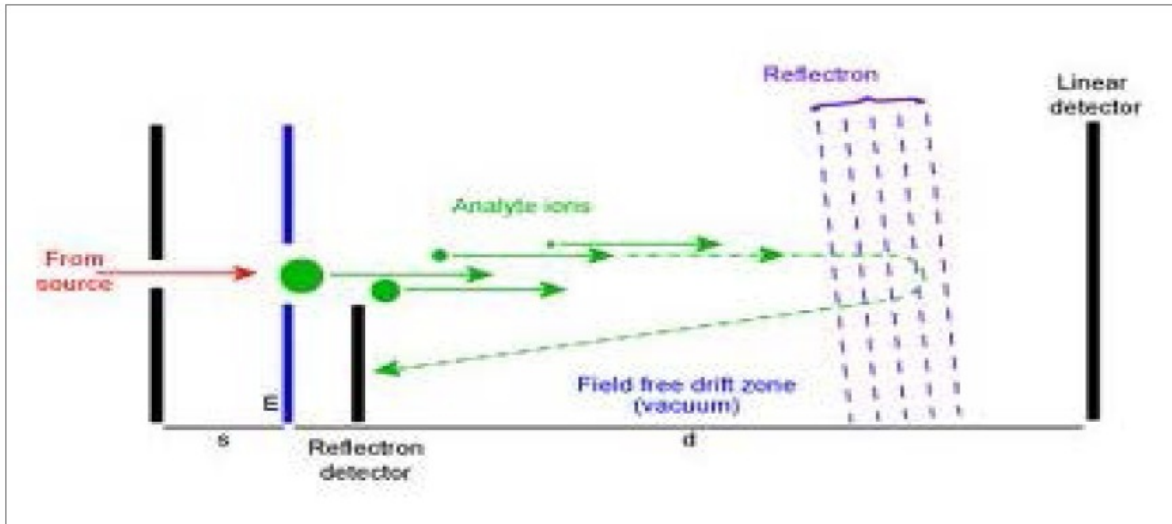
4- Detectors:

A time of flight (TOF) detector can discriminate between a lighter and a heavier elementary particles of same momentum using their time of flight between two detectors.

Two detectors are used in TOFMS to measure the time of flight
1. To indicate the time of production of ion(*channeltron*)
2. To indicate the time of collection(*Micro channel plate*)

Micro channel Plate:

A **micro-channel plate (MCP)** is a planar component used for detection of particles (electrons or ions) and impinging radiation (ultraviolet radiation and x rays). It is closely related to an electron multiplier, as both intensify single particles or photons by the multiplication of electrons via secondary emission. However, because a micro channel plate detector has many separate channels, it can additionally provide spatial resolution.

A micro-channel plate is a slab made from highly resistive material of typically 2 mm thickness with a regular array of tiny tubes or

slots (micro channels) leading from one face to the opposite, densely distributed over the whole surface.

The micro-channels are approximately 10 micrometers in diameter and they are parallel to each other and often enter the plate at a small angle to the surface (~8° from normal). The flat end plates are coated with a metallic alloy so that a potential difference can be maintained along the length of the channel.
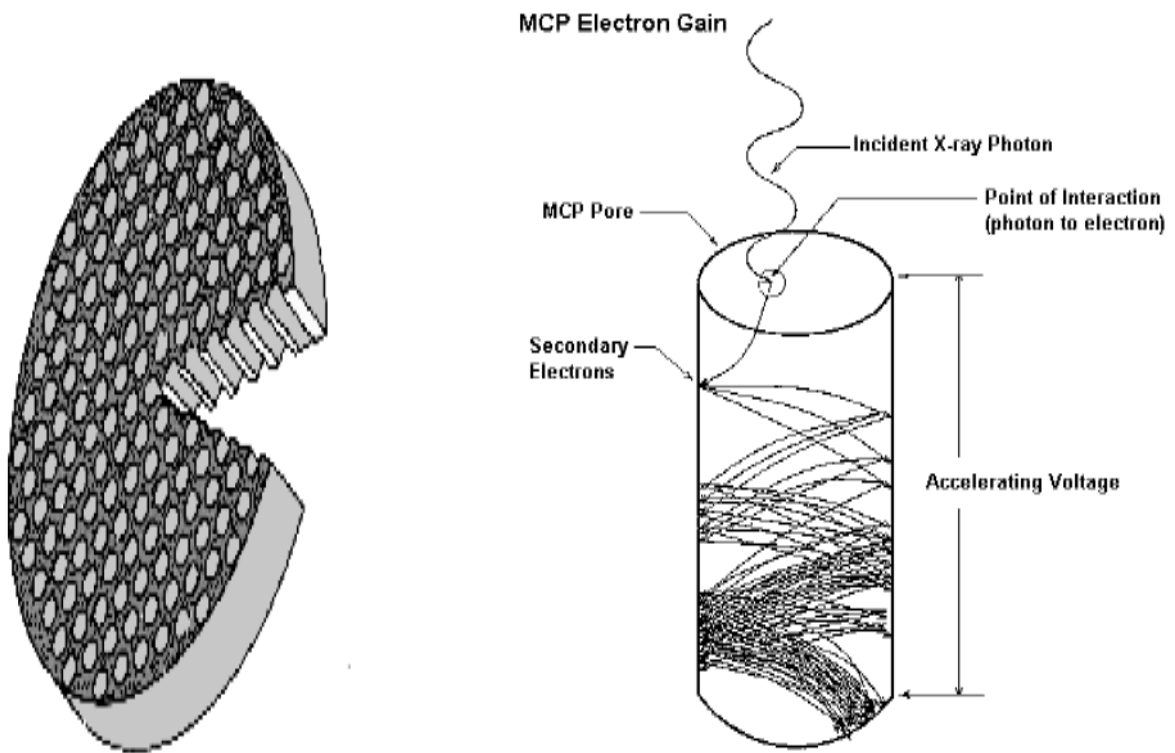
Most modern MCP detectors consist of two micro channel plates with angled channels rotated 90° from each other which is known as *chevron configuration.*

Operation:

Each micro channel is a continuous-dynode electron multiplier, in which the multiplication takes place under the presence of a strong electric field. A particle or photon that enters one of the channels through a small orifice is guaranteed to hit the wall of the channel due to the channel being at an angle to the plate and thus the angle of impact. The impact starts a cascade of electrons that propagates through the channel, which amplifies the original signal by several orders of magnitude depending on the electric field strength and the geometry of the micro-channel plate(approximately 10^6).
escape.
Typically, the dynodes are made of semiconductor material instead of metal since metals have a relatively high work function. A dynode consists of a secondary emission material deposited on a conducting material. A common technique is to form an alloy of an alkali or alkaline earth metal with a noble metal. Materials in common use are Ag-Mg, Cu-Be, and Cs-Sb. All of these have the requirements of a good dynode material:

Dynode materials and properties

The electron multiplier system amplifies the small current by causing a secondary emission to occur from the dynodes. This secondary emission is multiplied by the gain at each dynode stage, typically referred to as the secondary emission factor Δ. Secondary emission occurs via a process which is very similar to the photoelectric process. When an electron impacts on a dynode surface, energy is transferred directly to the electrons in the dynode material thereby allowing a number of secondary electrons to

1. high secondary emission - i.e. the average number of secondary electrons emitted per primary electron is high
2. stability of secondary emission effect under high currents
3. low thermionic emission, i.e. low noise

Calculation on TOF using C programming

```
// m - in kg
// E - in v
//Electric field - in v/m
// Distance - in m
// t-microsecond
//given Energy=5ev,Angle=30 Degree
```
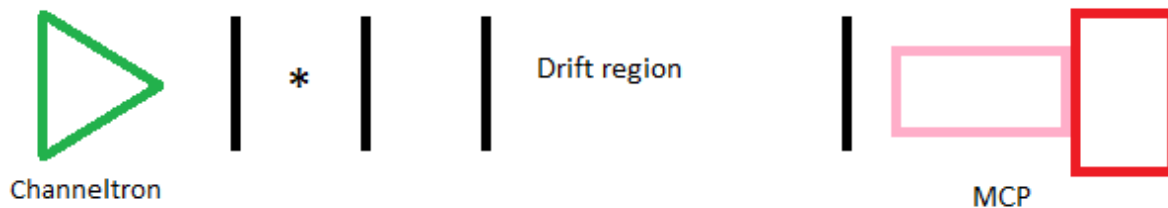


```c
#include<stdio.h>
#include<math.h>
#include<stdlib.h>     // Header file for srand and rand functions
#include<time.h>
void newton()
{
FILE *fp1;
 srand(time(NULL));            // Seed for random number     generator
      double T1,vs,vd,d,m,vmcp,as,ad,a;
      double D,us,U0,theta,ugiven;
      double q;
      double l,Tmcp,umcp,T0,s,Ts,Td,TD,T,rmcp,Vpos,Vs,Vd,VD,Vmcp;
      double pi;
      int i,iSecret;
      pi=3.141593;
      rmcp=.015;
      s=0.0095;    //half of the distance is considered where interaction happens
```

```c
        d=.114;
        D=.247;
        Vpos=161.54;
        Vs=-161.54;
        Vd=-2100;
        VD=-2100;
        Vmcp=-2150;
        m=(2.0)*1.67*pow(10,-27);                    //for deuteron
        q=1*1.6*pow(10,-19);
        U0=5*1.6*pow(10,-19);      // Energy

if((fp1=fopen("variationofangle5.dat","w"))==NULL)     // create a file for writing


     {
      printf("\n\n error opening output file \n");


     }



   for(i=0;i<100000;i++)
     {
      iSecret = rand() % 360 + 0;   // //   generate random number between 0 to 360
      theta =(float)iSecret;
      printf("theta =%f\n",theta);
      l=((theta*pi)/180);

    //  Calculation of TOF

   us=sqrt(2*U0)/sqrt(m);
   as=(q*(Vpos-Vs))/(m*2*s);
   vs=sqrt((us*us*cos(l)*cos(l))+(2*as*s));
//TOF in interaction region
   Ts=(vs-us*cos(l))/as;

ad=-(q*(Vd-Vs))/(m*d);
vd=sqrt(vs*vs+2*ad*d);
// TOF in acceleration region
td=(vd-vs)/ad;
```

```
// TOF in Drift region
TD=D/vd;
a=-(q*(Vmcp-VD))/(m*rmcp);
vmcp=sqrt(vd*vd+2*a*rmcp);
//TOF
Tmcp=(vmcp-vd)/a;
T=Ts+Td+TD+Tmcp;
T1=T*pow(10,6);
 fprintf(fp1,"%f %f\n",theta,T1);
  i=i+1;
}

fclose(fp1);
printf("\nOutput stored in variationofangle5.dat\n\n");
}
int main()
{
newton();
system("PAUSE");
return 0;
}
```
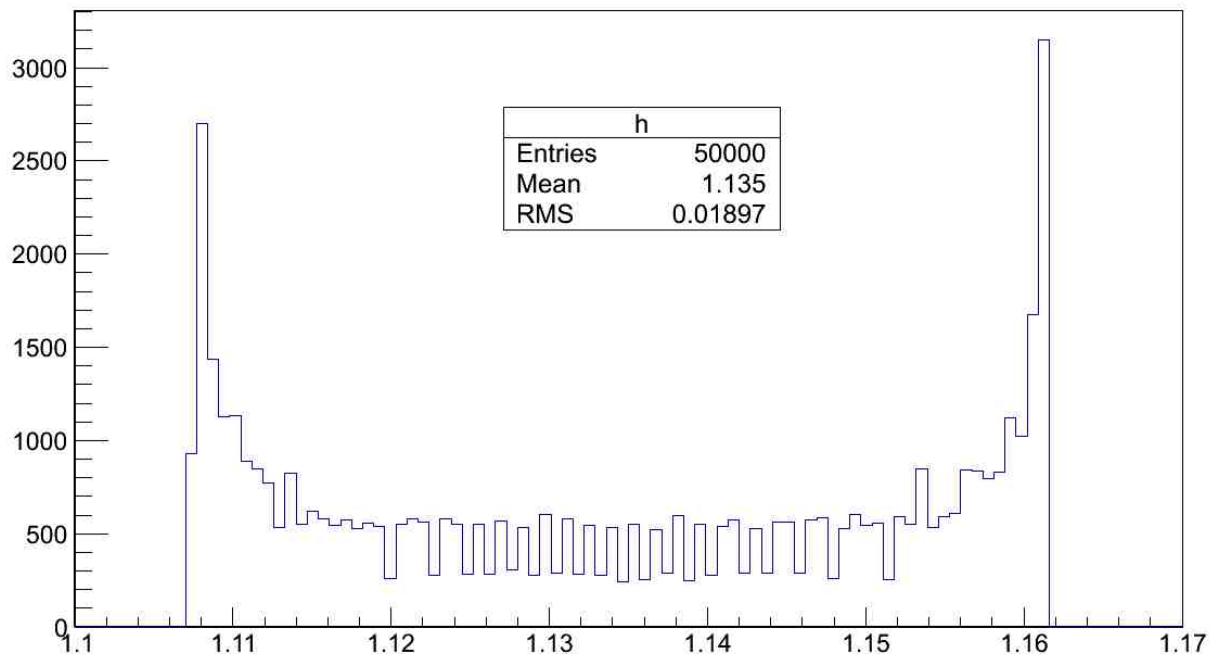
HISTOGRAM

This histogram shows that at the minimum time maximum number of particle reached at Detector and at the higher time maximum particle reached at the Detector. The histograms that result from executing above program are as shown:

Time 7

h	
Entries	50000
Mean	1.135
RMS	0.01897

SUMMARY

This work mainly aimed on the study about the information of different molecules. In this report I have noted down the basic information about TOFMS and written a C-program to generate a data by which I have made a time histogram by using ROOT. In starting section, I mentioned about the basic of TOFMS, MCP and Channeltron used in the experiment. Later part focused on the C-program and Histogram.