Analysis of Three-Body Breakup of Formic Acid Induced by a Strong Laser Field

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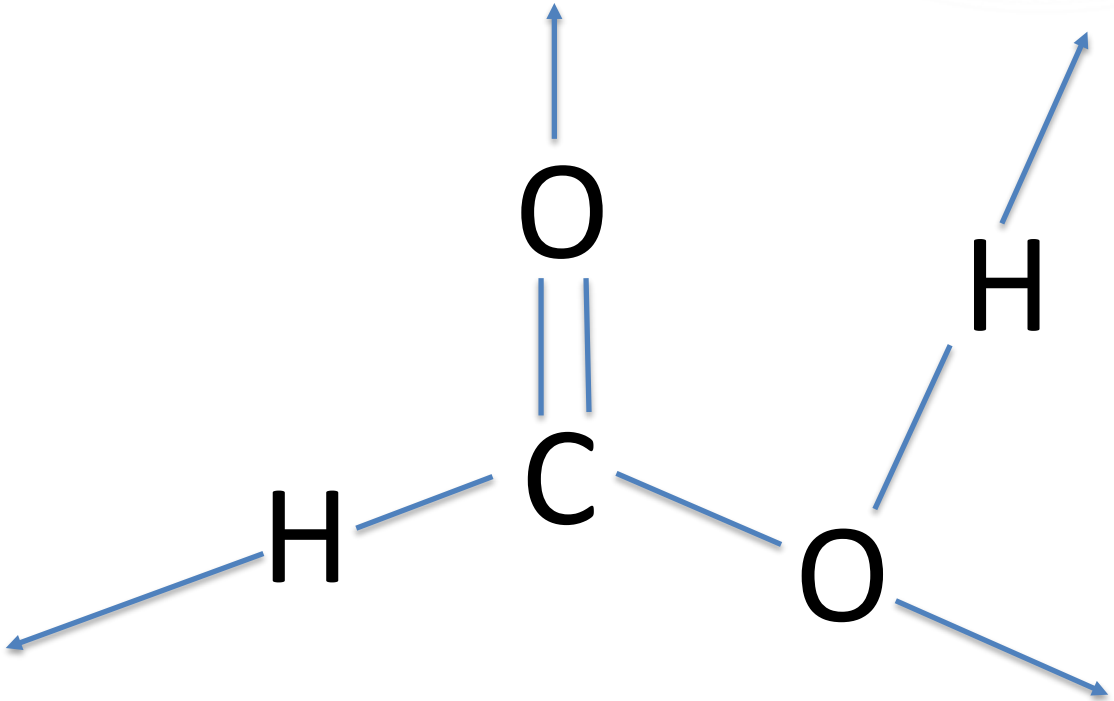
August 2, 2019

Ionization



The Inverse Problem

Inverse Method

Measured position and TOF data → Solving for breakup momenta → Understanding fragmentation dynamics

EEG or Electroencephalogram

[1] EEG. Digital Image. *MyDoctor.com.au,* 15, May 2013. https://www.mydr.com.au/tests-investigations/electroencephalogram-eeg

Types of Fragmentation

Concerted Fragmentation:

$$ABC \rightarrow A + B + C$$

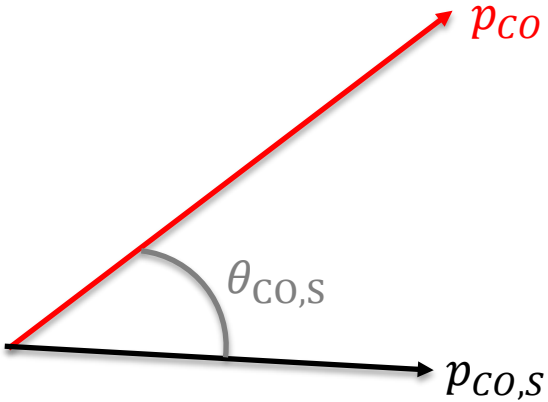
Sequential Fragmentation:

$$ABC \rightarrow AB + C \rightarrow A + B + C$$

Intermediate molecule

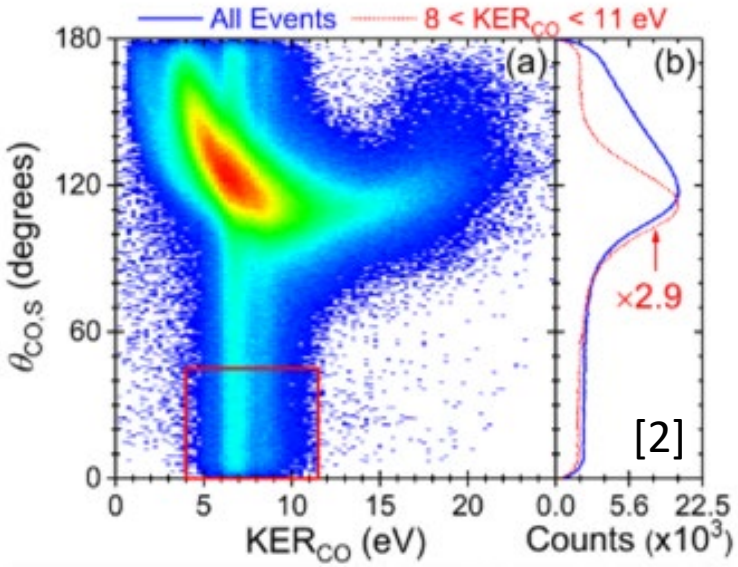
Plotting the Sequential and Concerted Breakup of Carbonyl Sulfide

$$OCS \rightarrow CO^{2+} + S^{+}$$
$$\rightarrow C^{+} + O^{+}$$



[2], [3]

If Sulfur breaks off first

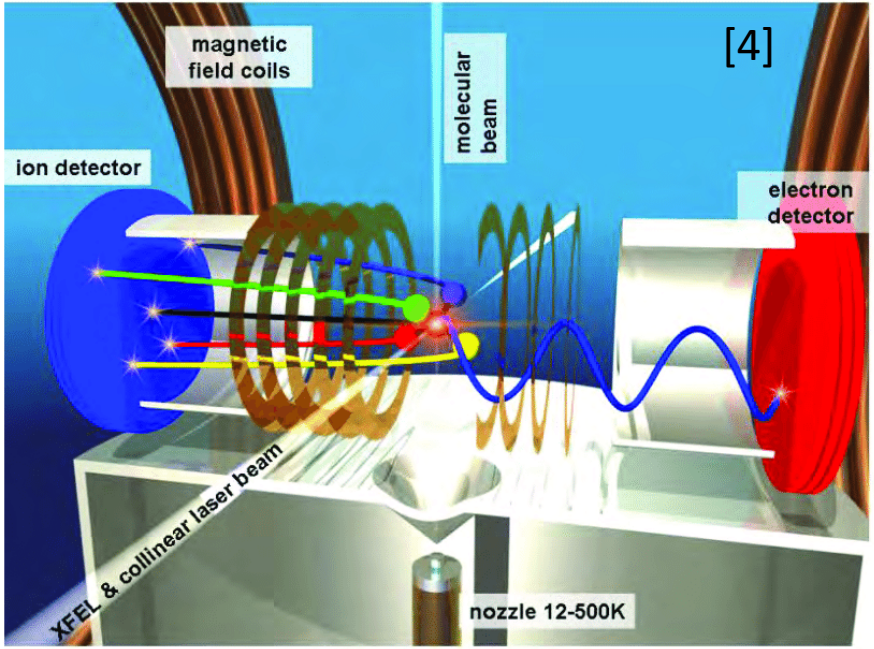


[2]: T. Severt, *et al.*, *Native frames: A new approach for separating sequential and concerted three-body fragmentation.* (2019)
[3]: Jyoti Rajput, *et al.*, 120, 10. (2018)

The Experiment

-**COLTRIMS:** Cold Target Recoil Ion Momentum Spectrometry

-my role: analyze the three body fragmentation of formic acid and look for sequential fragmentation



[4]: COLTRIMS. Digital Image. *Roentdek.com,* http://www.roentdek.com/Coltrims/

Formic Acid or HCOOH

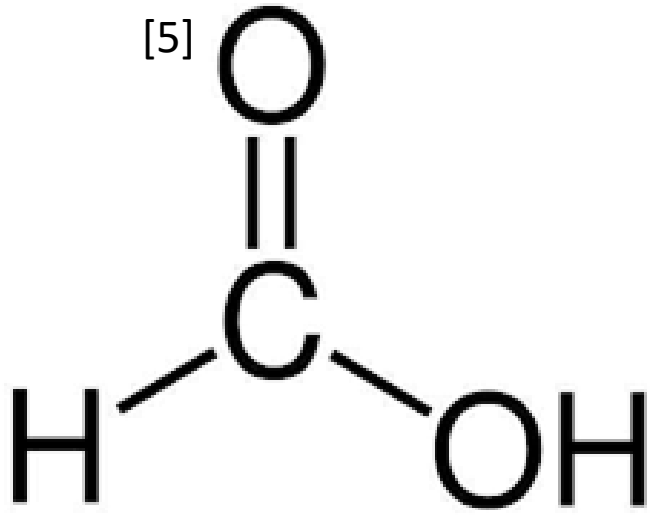
-Example Three Body Channel:

$$H^+ + HCO_2^{2+}$$
$$\rightarrow H^+ + CO^+ + OH^+$$

or

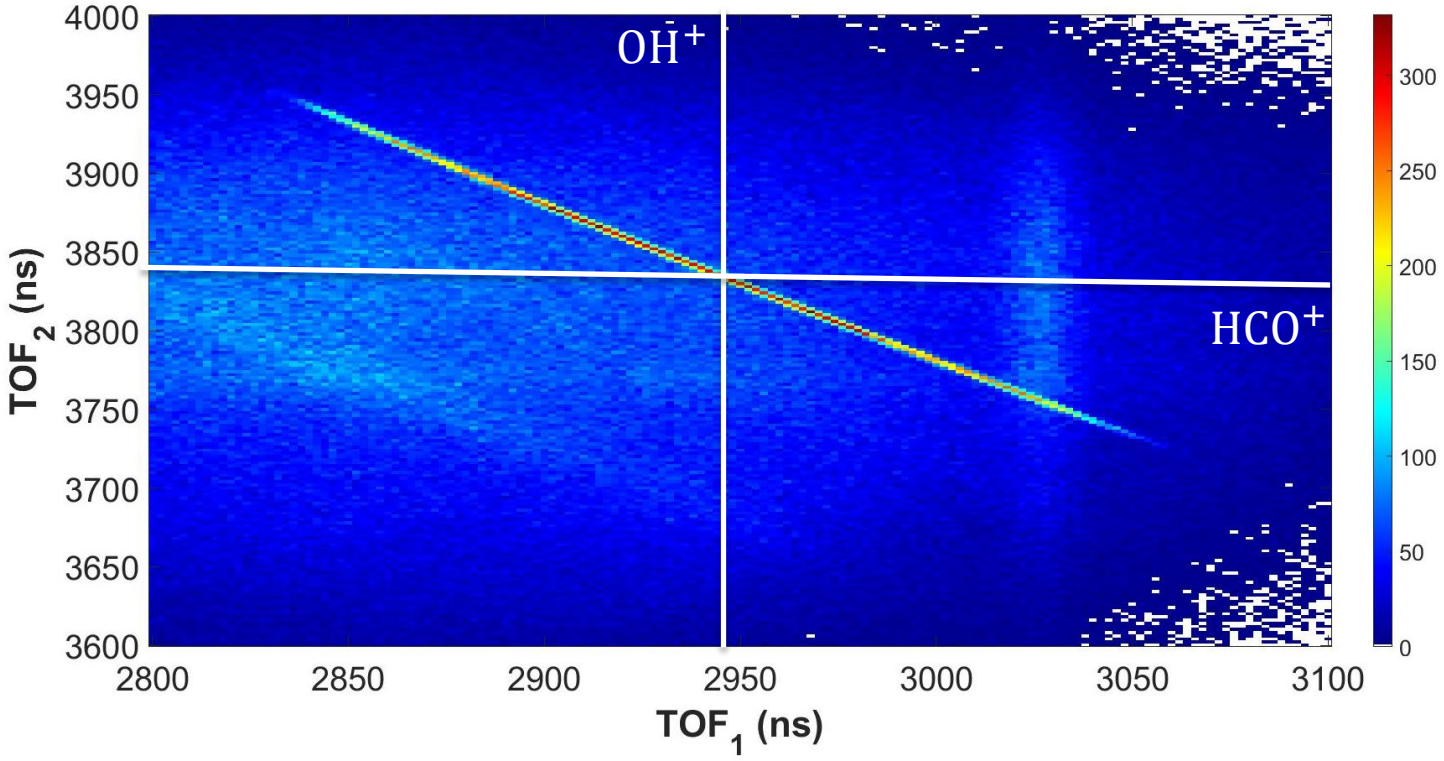
$$\rightarrow H^+ + H^+ + CO_2^+$$

[5]

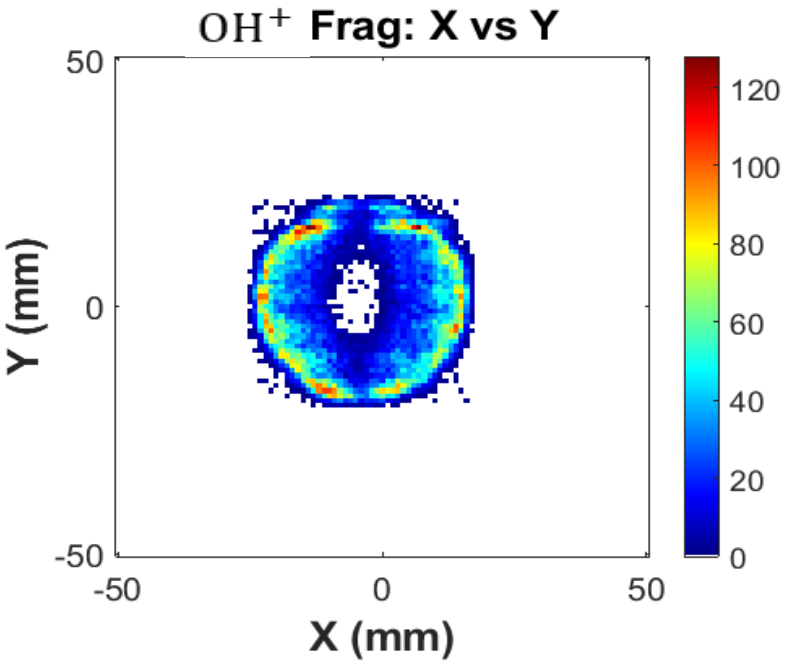


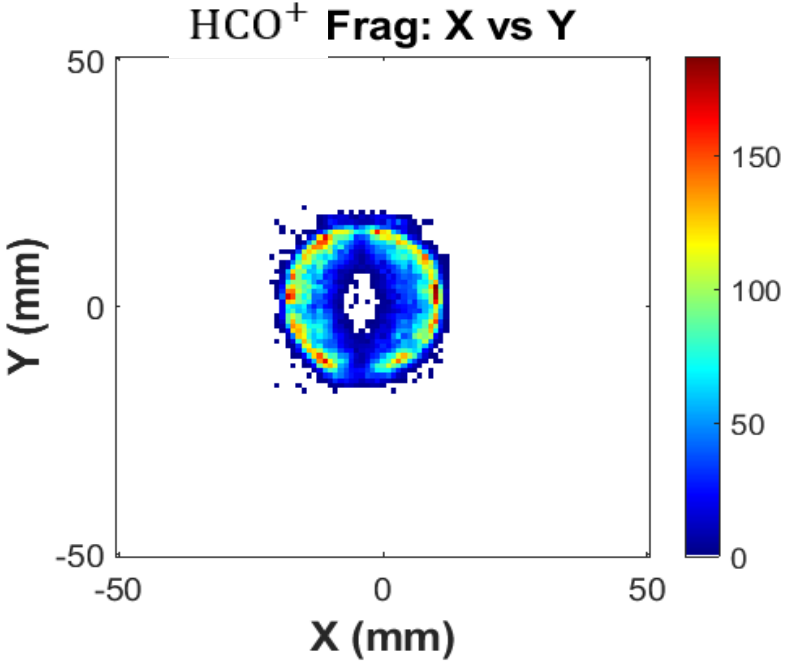
[5] Formic Acid. Digital Image. *Quora.* 4 July, 2019, https://www.quora.com/What-is-the-formula-of-methanoic-acid

Two Body Breakup Channels



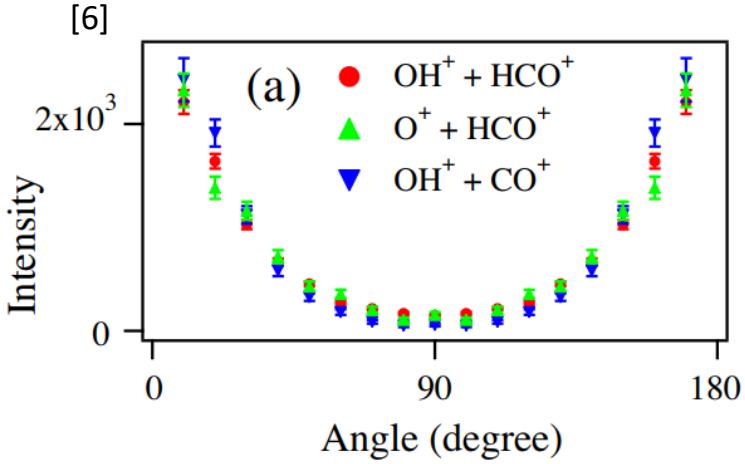
Problems with the Detector



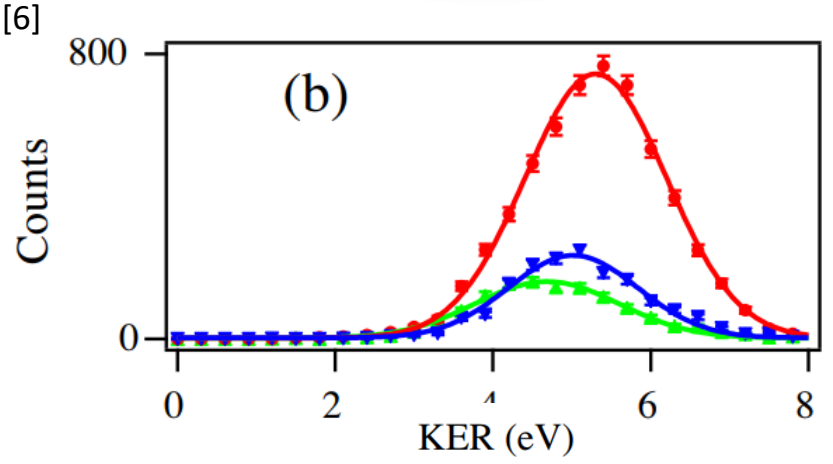


Digitizing Data from Wang *et al*. [6]

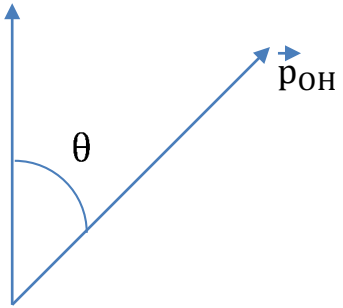
[6]

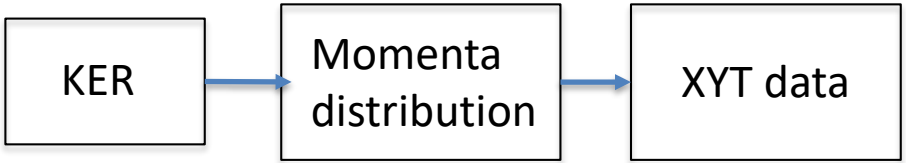


[6]



Laser polarization





[6] C. Wang *et al.*, Chem. Phys. 430, 40 (2014).

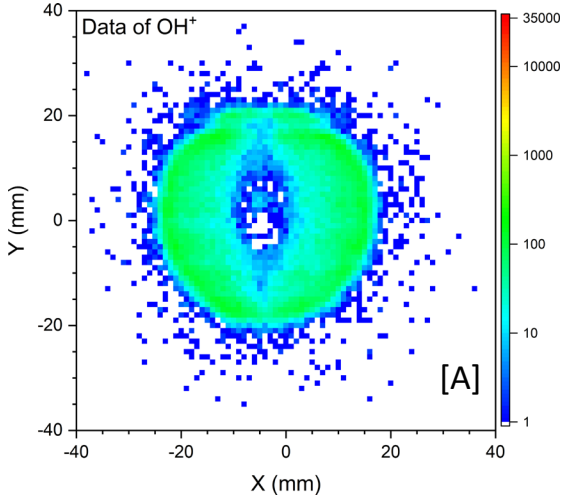
Calculating Efficiency of the Detector

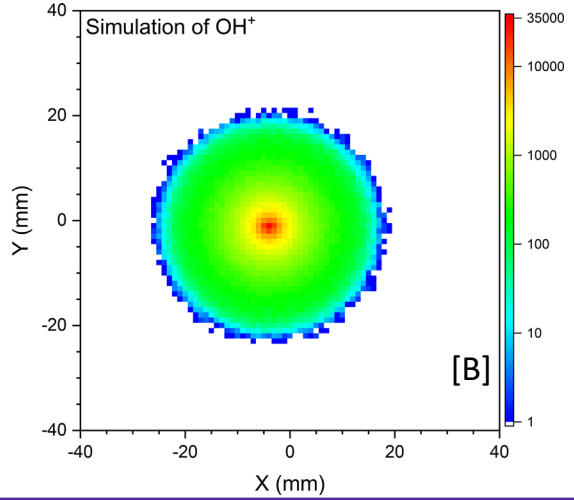
$$A = \epsilon B$$

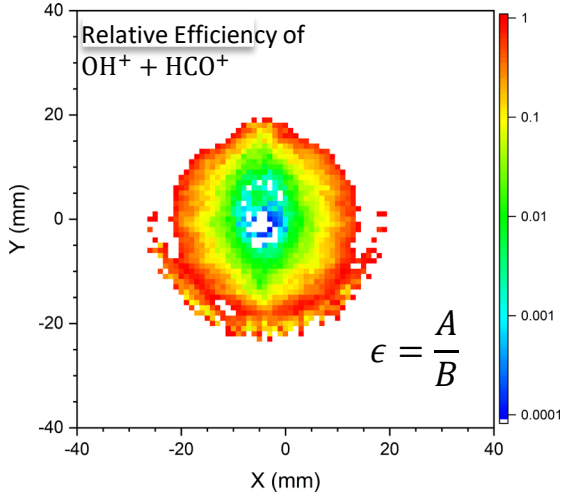
Measured data

Efficiency

Simulated experimental data

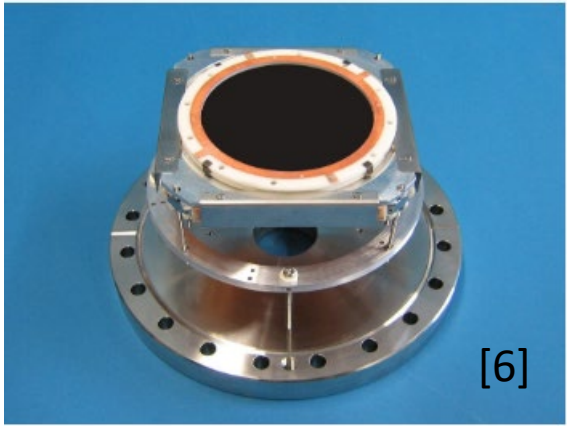






Future Outlook

- The efficiency calculation method can be recreated for similar experiments
- In order to successfully perform this experiment, it would be necessary to use new MCP plates



[6]: MCP Delay Line Detector. Digital Image. *Roentdek.com,* http://www.roentdek.com

Acknowledgements

Dr. Itzik Ben-Itzhak
Travis Severt
Dr. Daniel Rolles
Dr. Artem Rudenko
Farzaneh Ziaee
Kurtis Borne

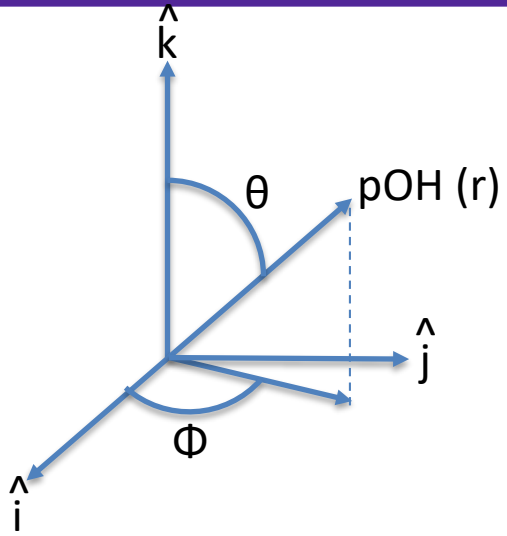
Dr. Loren Greenmen
Dr. Bret Flanders

National Science Foundation
James. R. Macdonald Laboratory
U.S. Department of Energy
Kansas State University

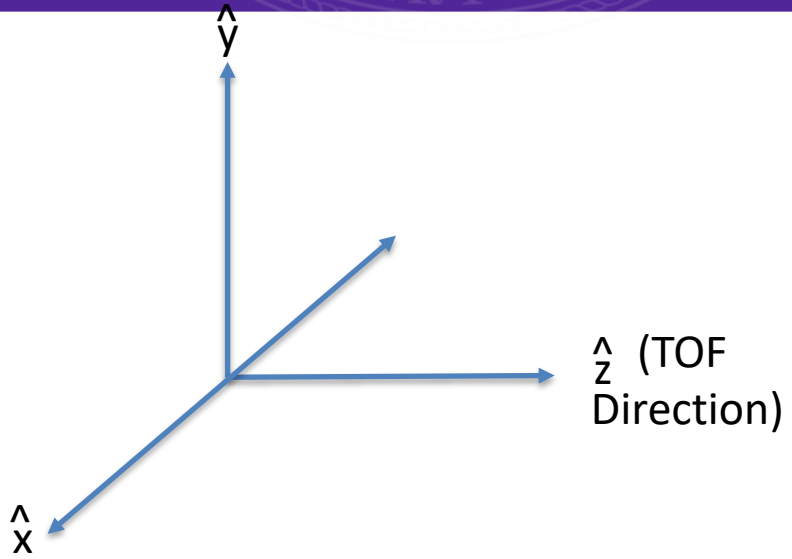
Digitization Process

- Calculated magnitude of momentum from KER
- Get the momenta distribution in the XYZ directions
- Solve imaging equations from our experimental set up to get XYT data
- Use theta and phi distribution to get angular distribution

Converting Digitized Data to XYT Data



First we convert from polar to cartesian coordinates.

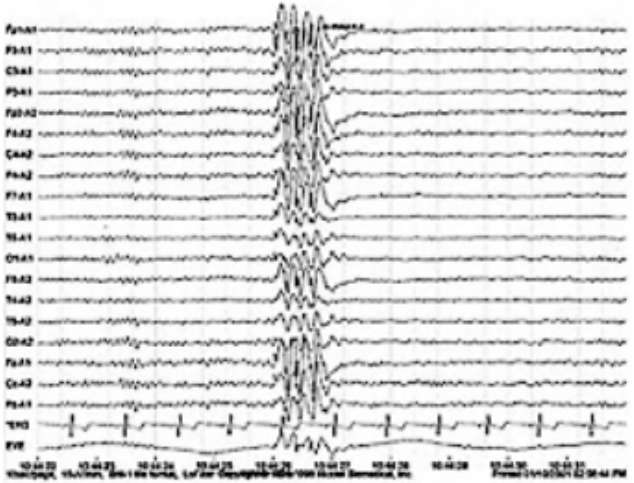


Then, we convert to the coordinates of our experiment: XYT

EEG as an Inverse Problem

Electrodes on the head to detect brain waves

EEG. Digital Image. imotions.com, https://imotions.com/blog/what-is-eeg/



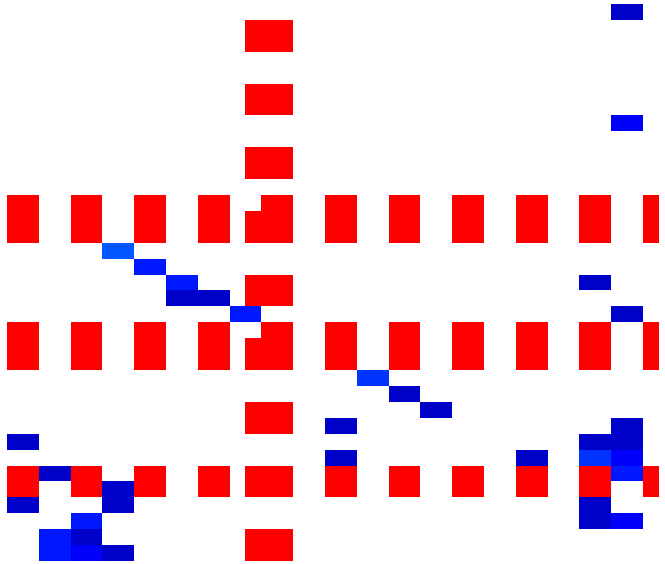
Sample EEG recording

EEG Scan. Digital Image. mayfieldclinic.com, https://mayfieldclinic.com/pe-eeg.htm

Background of OH+ HCO+ Channel

-

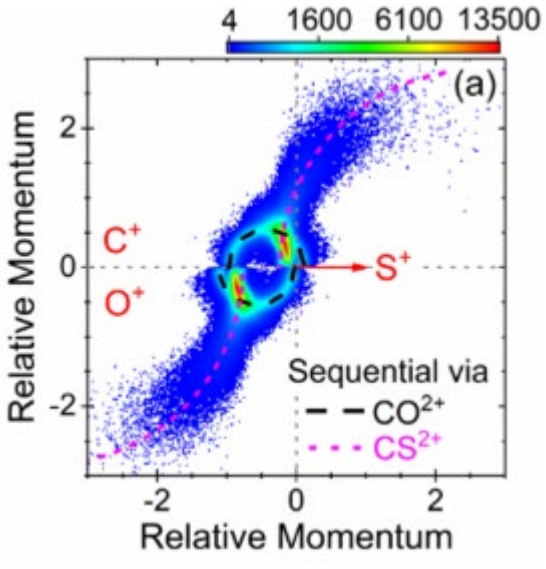
HCO+



OH+

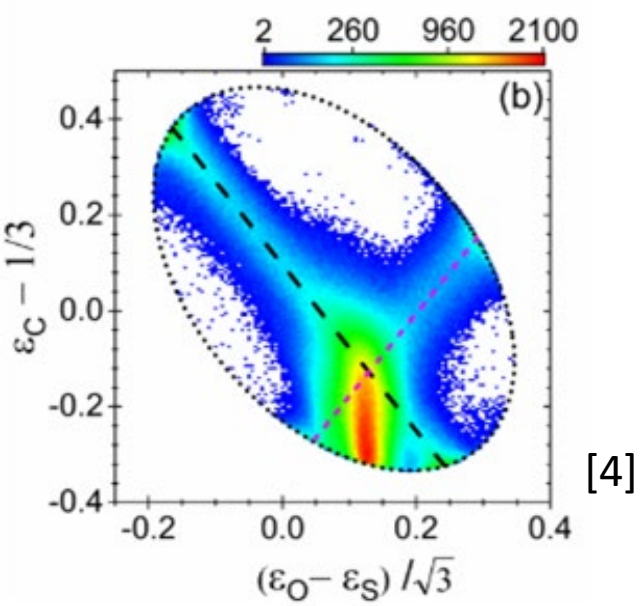
Newton Diagrams and Dalitz Plots for three body breakup of OCS into O+C+S+

Newton Diagram



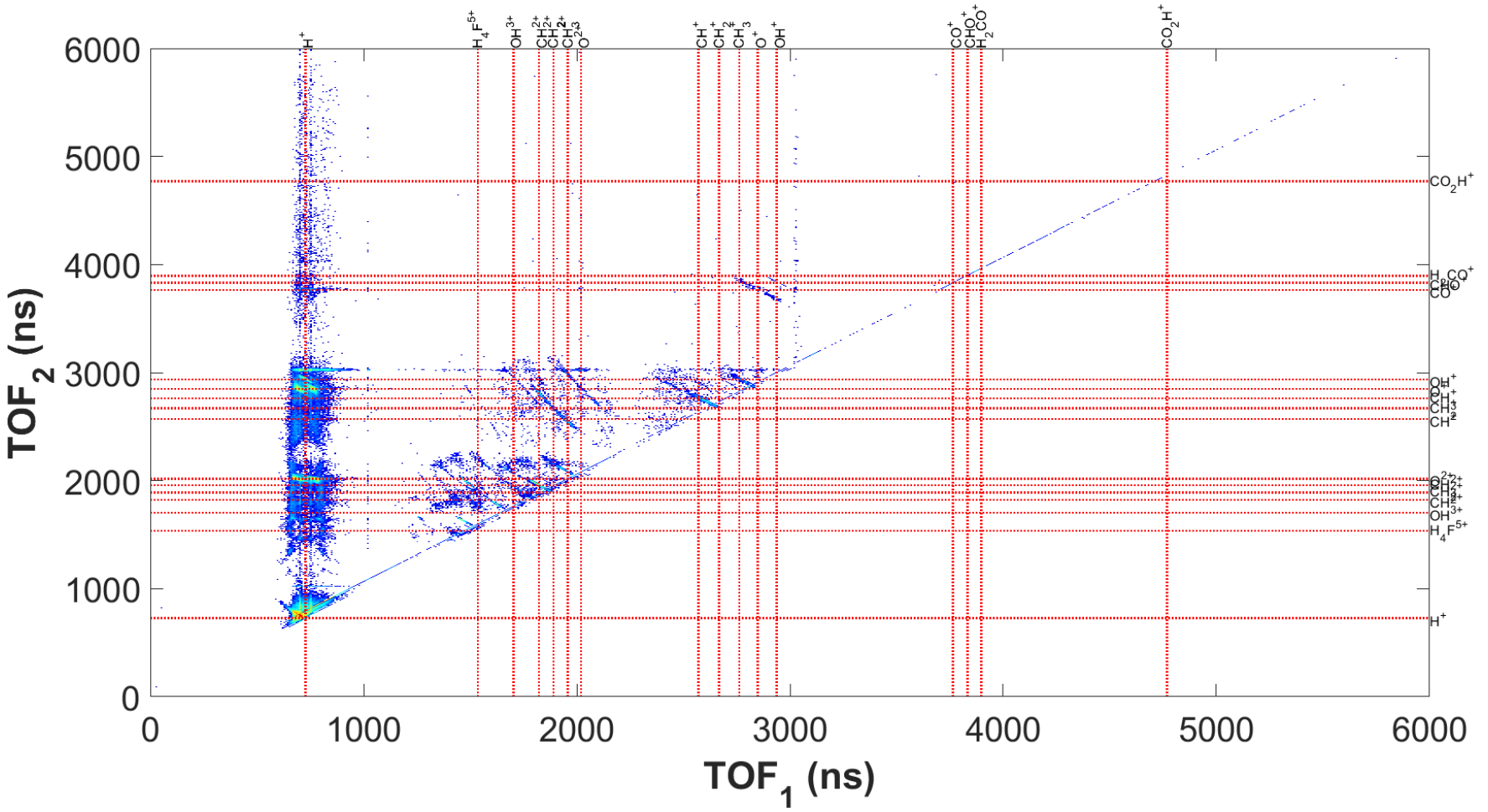
[4]

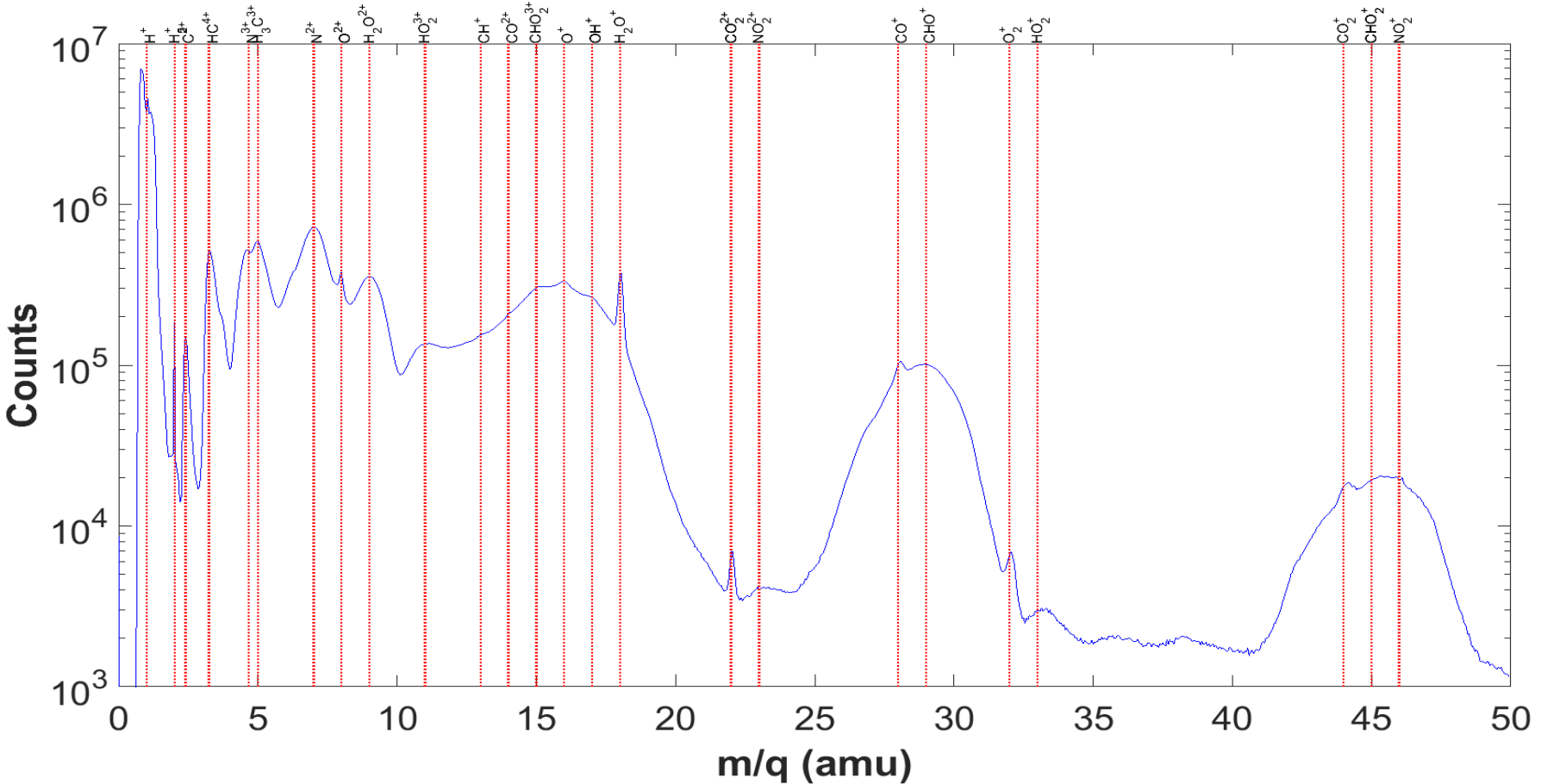
Dalitz Plot



[4]

[4]: T. Severt, et al., *Native frames: A new approach for separating sequential and concerted three-body fragmentation (2019)*


TOF2 (ns)
TOF1 (ns)
0
1000
2000
3000
4000
5000
6000
H+
H4F5+
OH3+
CH22+
CH2+
CH2+
O2+3
CH+
CH+2
CH3
O+
OH+
CO+
CHO+
H2CO+
CO2H+
CO2H+
H2CO+
CHO+
CO+
OH+
CH+
CH+2
CH3
CH2+
O2+
CH22+
CH2+
CH2+
OH3+
H4F5+
H+


Counts
m/q (amu)
10^7
10^6
10^5
10^4
10^3
0
5
10
15
20
25
30
35
40
45
50
H^+
H_2^+
C^{4+}
HC^{4+}
N_3^{3+}
C^{3+}
N^{2+}
O^{2+}
H_2O^{2+}
HO_2^{3+}
CH^+
CO^{2+}
CHO_2^{3+}
O^+
OH^+
H_2O^+
CO_2^{2+}
NO_2^{2+}
CO^+
CHO^+
O_2^+
HO_2^+
CO_2^+
CHO_2^+
NO_2^+

The Imaging Equations

-Used kinematics to derive equations for the momenta in each direction when there are N bodies (for N body breakup)

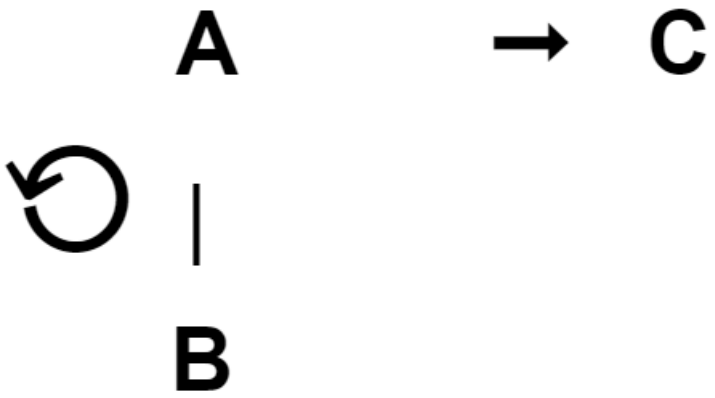
$$p_{Nx} = m_N\left(\frac{x_N - x_0}{t_N} - \frac{1}{\sum_{i=1}^{N} m_i}\left(\sum_{i=1}^{N} \frac{x_i - x_0}{t_i}\right)\right)$$

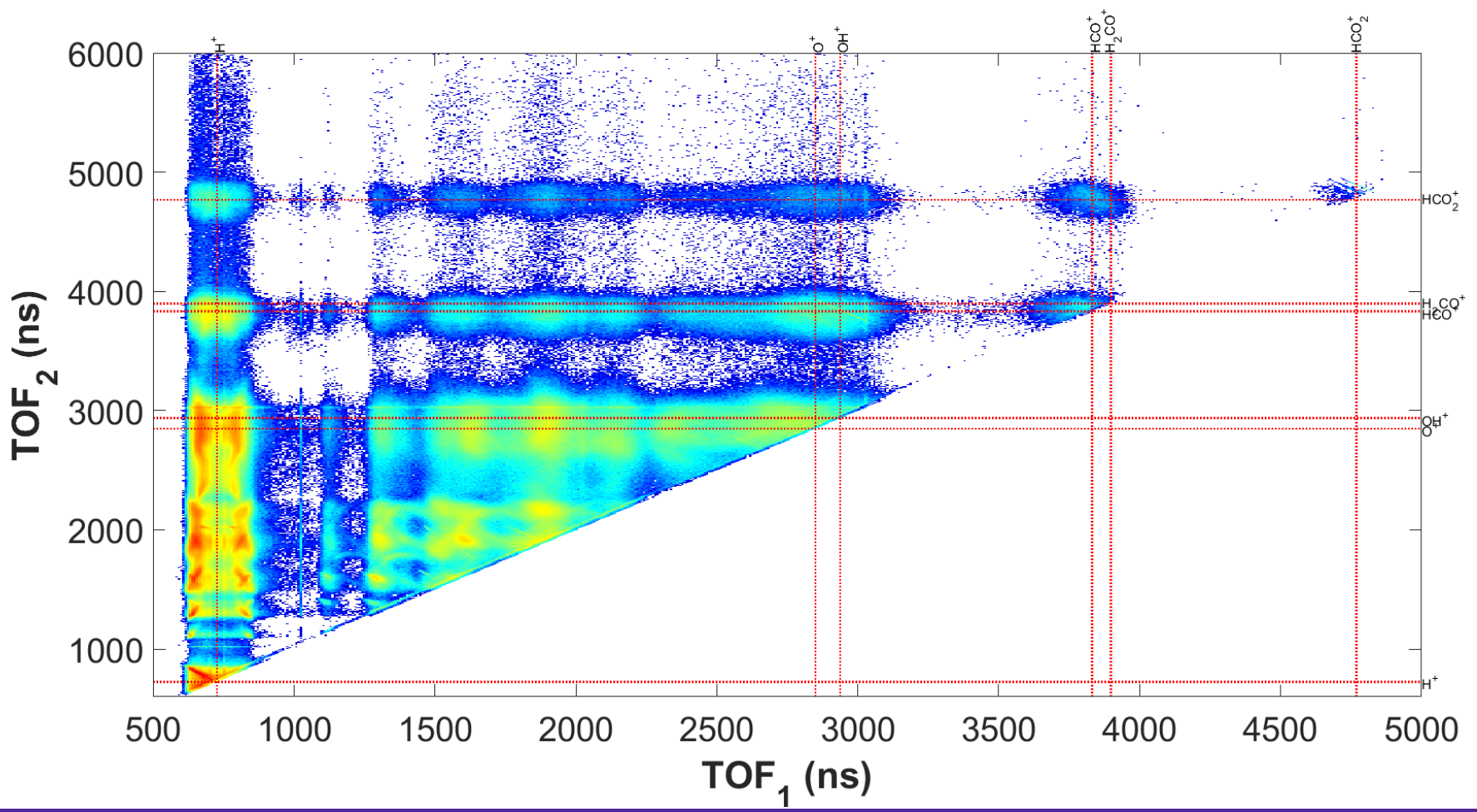
$$p_{Ny} = m_N\left(\frac{y_N - y_0}{t_N} - \frac{1}{\sum_{i=1}^{N} m_i}\left(\sum_{i=1}^{N} \frac{x_y - y_0}{t_i}\right)\right)$$

$$p_{Nz} = m_N\left(\frac{l - z_0}{t_N} - \frac{a_N}{2t_N} - \frac{1}{m_{mol}}\sum_{i=1}^{N}\left((m_i)\left(\frac{l - z_0}{t_i} - \frac{a_i t_i}{2}\right)\right)\right)$$

Our Analysis Method

-We can use basic mechanics to observe the fragmentation process of any molecule




H+
O+
OH+
HCO+
H2CO+
HCO2+
HCO2+
H2CO+
HCO+
OH+
O+
H+
6000
5000
4000
3000
2000
1000
TOF2 (ns)
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
TOF1 (ns)