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Verslag van de korte stage op het KVI bij de Atomic Physics Group. Begleiding door drs. F. Alvarado en onder leiding van prof. dr. R. Morgenstern, prof. dr. ir. R. Hoekstra en dr. Thomas Schlathölter.

Abstract

Ionization and fragmentation of the amino acid glycine upon interaction with He^{2+} ions has been studied. By means of time-of-flight spectroscopy the fragments have been analyzed. Goal was to identify temperatures at which the glycine molecule vaporizes without being thermally dissociated. It was found that in the region of 145 °C to 180 °C the glycine molecule vaporizes without thermal dissociation. Future measurements are recommended to be done at temperatures between 160 °C and 180 °C. A fragment coincidence measurement has also been performed. This showed coincidence of fragments such as H^+ , CH^+ , N^+ , NH_4^+ , HCNH^+ , NH_2CH_2^+ , HOCO^+ and others. Insufficient statistics allowed only one kinetic energy release (KER) estimation to be made, which was found at 6.3 μeV and too small to be correct.

Introduction

Radiation damage occurs daily to everyone. Radiation sources can vary: background radiation from the universe, from radioactive elements like Uranium or in a hospital when radiation is used for treatment of a tumor [1].

Cells can get damaged or even killed by radiation. This can be a result of biomolecules being fragmented. DNA is particularly vulnerable to radiation damage. Damaged DNA can be repaired, but sometimes it is repaired wrong. This can lead to chromosomal abnormalities and mutations [2]. Radiation can also interact with the cellular water, causing ion radicals to be formed, which then attack the DNA [2].

Therefore, investigating the effects of radiation on biomolecules is very important. There are several applications.

For one, it is of importance to know how cells take damage, which biomolecules are vulnerable to what kind of radiation components. This knowledge can be used in the medical world. For instance, to know what kind of damage has been done in case of a radiation accident. But more important, knowledge about this subject can be used in radiotherapy. The goal of radiotherapy is to kill cancer cells without damaging other cells [1]. Not just Röntgen radiation is being used here, but also electrons and ions.

This is where our research comes in. We study the behavior of various biomolecules including but not limited to: adenine, glycine, adenosine, desoxyribose, uracil and thymidine [4][6].

In addition, the research that was performed has a fundamental value: how these biomolecules respond to several forms radiation is not fully known yet.

This particular paper is about radiation damage to glycine.

Glycine

Chemical formula: $C_2H_5NO_2$.
Molecular mass: 75.07 g mol^{-1}
Structural build:



Fig. 1.1: The structural build of glycine, 2D (left) and 3D (right)

Glycine is an amino acid. Amino acids are a part of certain proteins. Proteins are built from 20 different amino acids [7]. This is not just valid for the human body; proteins built from the same 20 amino acids are found in all species. The genetic code contains information about the way proteins are built from amino acids. Proteins are essential to the structure and function of all cells.

All amino acids are of the following form:

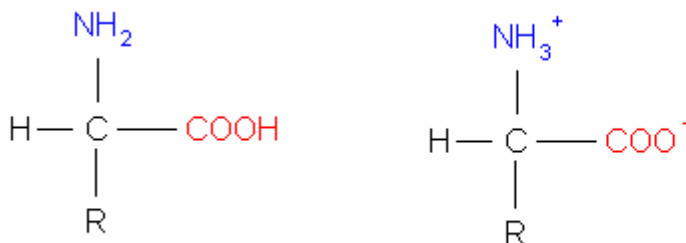


Fig. 1.2: Standard amino acid groups. The normal form is shown at the left, on the right the dipolar form.

They all have an amine group (NH₂), a carboxyl group (COO), a hydrogen atom and a side chain, denoted by R here. It is the side chain that defines the amino acid.

There is one structural exception to this. In proline, the side chain has a bond with the carbon atom as well as with the hydrogen atom.

Amino acids in solution at neutral PH are mostly of the dipolar ion (or: zwitterion) form. The dipolar form is shown on the right in fig.1.2. In the dipolar ion form of an amino acid, the amino group is protonated (NH₃⁺) and the carboxyl group is dissociated (COO⁻). At very low PH (around 2 or less), the amino group is ionized (NH₃⁺), while at very high PH (10 or higher) the carboxyl group is ionized (COO⁻)

In case of glycine, the side group consists of one hydrogen atom. This makes glycine the simplest of all amino acids.

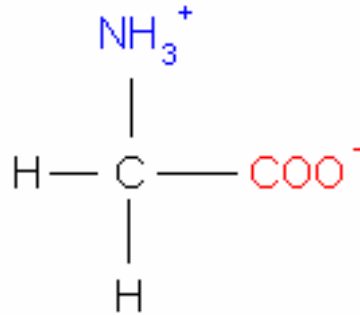


Fig. 1.3: *Glycine, dipolar form*

Most proteins contain a small amount of glycine, except for collagen. One third of collagen consists of glycine. This is due to geometrical reasons: the only amino acid that fits as residue near the helix axis is glycine. Other amino acids are too large to fit in.

Experimental setup

ECRIS

The ions used in our experiment were generated in the Electron Cyclotron Resonance Ion Source (ECRIS) at the Atomic Physics department. The ECRIS is floated on potentials from 1 kV to 25 kV. During this experiment, a potential of 10 kV was used for He^{2+} ions. The principle of the ECRIS operation can be described as follows.

Highly charged ions are produced stepwise by electron impact ionization. During bombardment by electrons, ions or atoms are subsequently ionized. These electrons are produced inside a magnetic trap.

This trap, a radial hexapole magnet and two axial magnet coils, consists of magnetic fields increasing in all directions. Electrons move inside the trap with a revolution frequency ω_c . High energy electrons are produced by applying a radiofrequency (RF) field. When the RF frequency matches ω_c , electron cyclotron resonance occurs. The electrons are resonantly accelerated by the RF field.

After passing a 110° magnet for m/z separation, a system of quadrupole magnets triplets and bending magnets guide the projectile ion beam into the collision region. By means of correction magnets, the shape of the beam can be modified until an optimal and stable current is acquired.

CHEOPS

Before entering the collision region, the beam passes the Chopper Sweeper system (see Fig. 2.1). The function of this system is to chop the ion beam in small pulses. This was done by keeping one chopper plate constant at a voltage of 100 V, and a second one oscillating between 0 and 200 V. This produces ion pulses of a few ns. During the experiment, the chopper sent pulses of 36 μs , with a period of 72 μs .

The pulsed beam then enters the collision region. In the collision region, there is glycine in gas form, evaporated from a 1-2 gram powder sample in the oven. The oven is heated by a resistor. Measurements at various temperatures (30°C to 180°C) were performed in order to find out at what temperature there is sufficient glycine in gas form, yet without thermally damaging the molecule. The oven is located about 20 mm from the collision center.

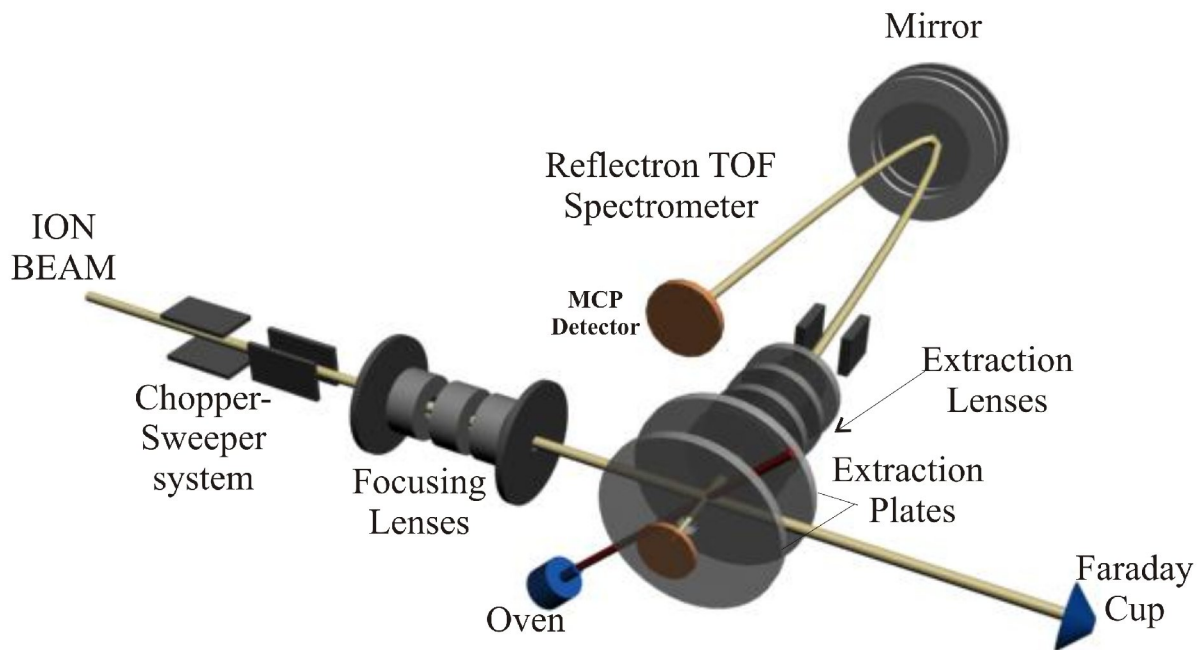


Fig. 2.1: Schematic view of the CHEOPS setup.

The collision region was held at a pressure around $1 * 10^{-8}$ mbar.

Behind the collision region is the Faraday Cup, which is used to measure the beam current.

The upper side of the collision region is a stainless steel plate which was cooled by liquid nitrogen. This serves as a trap for the residual gas.

This way, the contributions from background gasses are negligible.

The fragments produced during the collision are accelerated by a static homogeneous electric field of 600 V/cm, which is created by two plates that are 10 mm apart. The plates are resistively heated to approximately 100 °C, to avoid layers of glycine that can behave as insulating material, changing the electric field.

Because of this electric field, ions generated in the collision region are extracted through a diaphragm and a lens system into the reflectron time-of-flight (TOF) spectrometer and detected on a Micro Channel Plate (MCP) detector. The ions enter a fieldfree region, containing an electrostatic mirror to reflect them into the MCP detector. The length of the reflectron path is 160 cm. Using the reflectron TOF spectrometer, the ratio of mass and charge (m/z) can be measured.

Heavy ions with low charge will travel relatively slow, and light ions with high charge will travel fast. This can be seen from the following formula that relates flight time, mass and charge:

$$t = \frac{s}{v} = s \sqrt{\frac{1}{2} V \frac{m}{z}} \quad (2.1)$$

Where s is the distance, V is the accelerating potential, v is the speed, m is the mass and z is the charge.

The time of flight is proportional to the square root of m/z.

The signal from the MCP detector goes to a preamplifier and then to an amplifier, after that to a discriminator and after it is filtered, it goes to a time to digital converter. The time to digital converter is connected to a PC (FAST ComTec P7888, 1 ns resolution).

The objective of the present study is to measure glycine TOF spectra at different temperatures to identify the range of temperatures where the fragmentation pattern does not change anymore.

Kinetic energy calculation

The kinetic energy of fragments can be calculated by using the TOF data. Assuming a two-body breakup, the law of conservation of momentum tells us that the two fragments travel in opposite direction after the collision. One travels towards the detector, and away from it. Because of the extraction plates, the ion emitted away from the detector, will be accelerated in the opposite direction until it's back in initial position. The time in which this is done, is equal to Δt . This time difference can be seen between two peaks in one island. The time difference is equal to:

$$\Delta t = \frac{\sqrt{8\mu U_{\text{ker}}}}{qE} \quad (2.2)$$

Where μ is the reduced mass:

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \quad (2.3)$$

U_{ker} is the Kinetic Energy Release, q is the charge state and E is the extraction field strength.

This means the KER can be calculated as follows:

$$U_{\text{ker}} = \frac{(\Delta t q E)^2}{8\mu} \quad (2.4)$$

Error analysis

The statistical counting error is proportional to the number of counts, N [12].

When calculating the ratio between two specific peaks, the error is calculated as follows. Independent errors that are processed through a function $f(x,y)$, with measurements x , y and their respective errors σ_x , σ_y sum up in the following manner:

$$(\sigma_f)^2 = \left(\frac{\partial f}{\partial x}\right)^2 (\sigma_x)^2 + \left(\frac{\partial f}{\partial y}\right)^2 (\sigma_y)^2 \quad (2.5)$$

When calculating a ratio, the function f has the following form:

$$f = \frac{x}{y}$$

This means that the error in the ratio is:

$$\sigma_f = \sqrt{\left(\frac{\sigma_x}{y}\right)^2 + \left(\frac{x}{y^2}\sigma_y\right)^2} \quad (2.6)$$

However, because $\sigma_x = \sqrt{x}$, this is reduced to:

$$\sigma_f = \sqrt{\frac{x}{y^2} + \frac{x^2}{y^3}} \quad (2.7)$$

Where σ_f is the error in the ratio, x is the integral of the first peak, and y the integral of the second peak.

Measurements

Four series of measurements were done. The first measurement series was to determine at what temperature the glycine fragments appeared. The second series explored the higher temperatures and the third was to obtain better statistics in the region where the glycine molecule vaporized. Temperatures varied from 30 °C to 180 °C.

The fourth measurement was a fragment-coincidence measurement. This was performed at a temperature of 165°C and with different chopper settings: pulses of 30 μ s with a period of 60 μ s.

Results and discussion

The first series of measurements was to find out at what temperature the molecule vaporized.

Because of the limited amount of time, the measurement time was relatively short and at T=150 °C the measurement had to be stopped.

This lead to the following results:

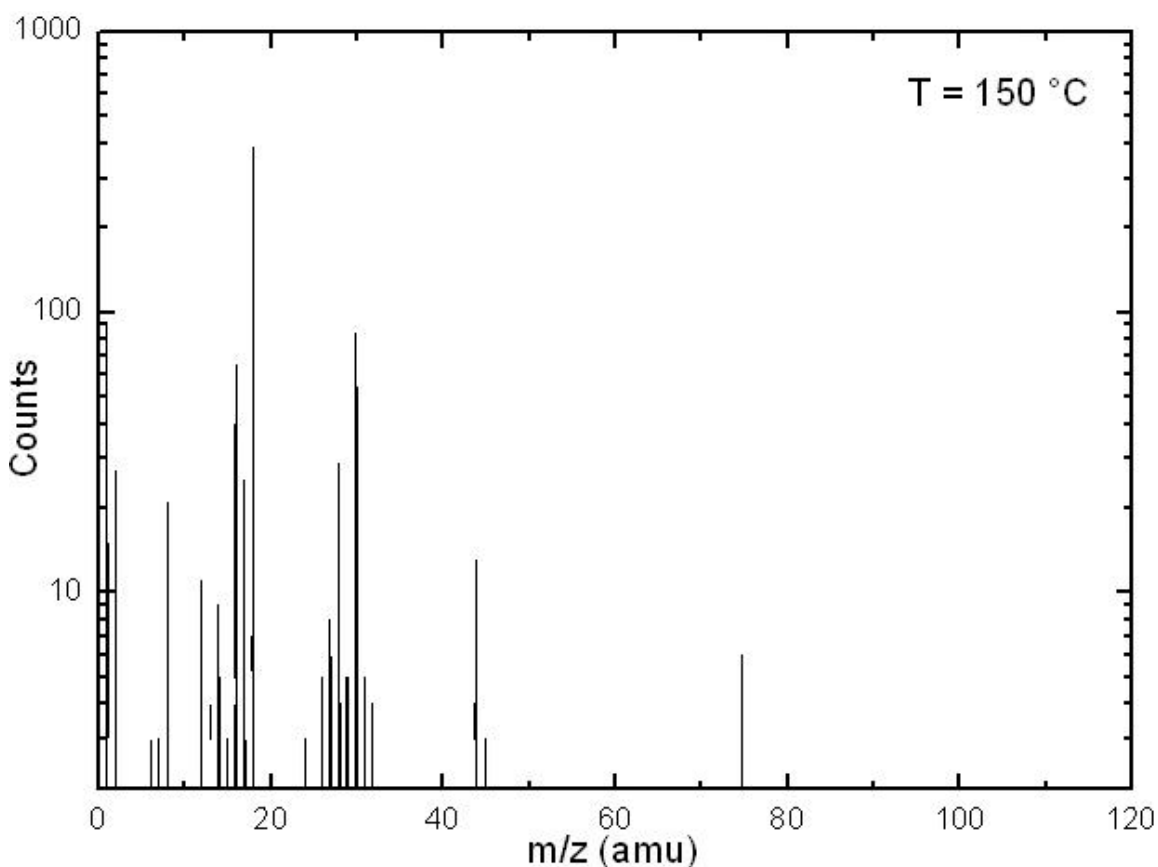


Fig. 3.1: Mass spectrum at $T = 150$ °C

Temperature (°C)	30	40	50	60	70	80	90	100	110	115	120	125	130	135	140	145	150
Peak size m/z=75 ¹	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0059	0.0065

Table 3.1: first measurement of the glycine molecule to determine the vapor temperature.

¹The peak sizes have been divided by the total integral to obtain a better picture

All measurements were done for a time interval of 300 seconds, except for the measurement at $T = 150\text{ °C}$. This was done for 500 seconds.

Glycine ($m/z = 75$) appeared from a temperature of 145 °C . It was, however, a very small peak with a total of only 34 counts. At $T = 150\text{ °C}$, the peak was larger, but still rather small with 55 counts. The increase is mainly because this particular measurement was done for 500 seconds instead of 300. But as can be seen from Fig 3.2, the glycine peak did increase relative to the total number of counts during the measurement.

Other researches with glycine give values such as 164 °C [9] and 155 °C to 165 °C [11] as evaporation temperature. There have also been reports of using a temperature between 150 °C and 200 °C to have enough target molecules but a temperature low enough not to damage the molecule [10]

During the next series of measurements, higher temperatures were explored. This lead to the following results.

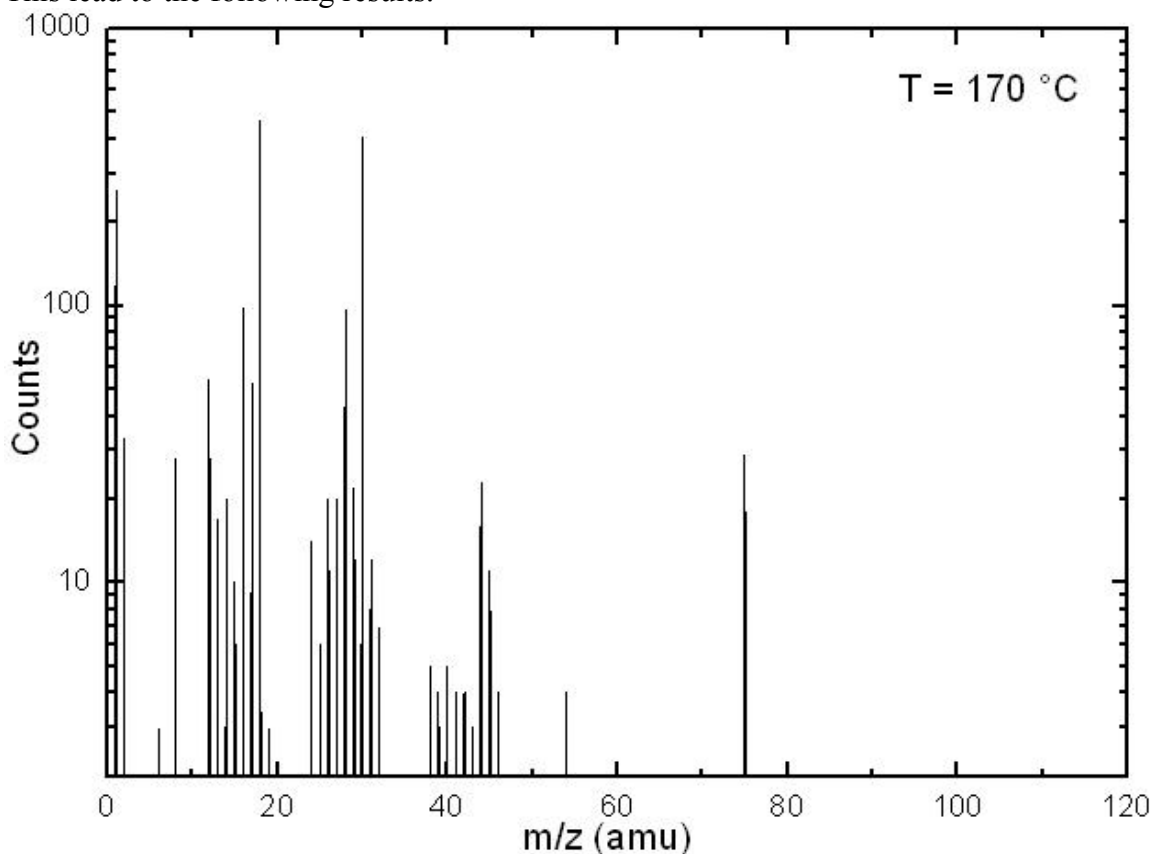


Fig. 3.2: Mass spectrum at $T = 170\text{ °C}$

Temp. (°C)	P _{cc} (mbar)	Time (s)	Ratio 30/75	Error 30/75	Ratio 28/75	Error 28/75	Ratio 12/75	Error 12/75	Ratio 12/30	Error 12/30	Size ¹ m/z=1	Size Error
95	7.31 * 10 ⁻⁹	300	-	-	-	-	-	-	-	-	0.034	0.009
100	7.15 * 10 ⁻⁹	600	-	-	-	-	-	-	-	-	0.046	0.007
105	7.16 * 10 ⁻⁹	300	-	-	-	-	-	-	-	-	0.041	0.007
110	7.18 * 10 ⁻⁹	300	-	-	-	-	-	-	-	-	0.041	0.009
130	9.37 * 10 ⁻⁸	300	-	-	-	-	-	-	-	-	0.053	0.009
150	1.91 * 10 ⁻⁸	300	-	-	-	-	-	-	-	-	0.085	0.008
160 [†]	3.48 * 10 ⁻⁸	300	11.9	2.4	4.5	0.9	2.1	0.5	0.18	0.03	0.079	0.005
170	5.18 * 10 ⁻⁸	600	16.7	1.0	5.0	0.3	2.0	0.2	0.122	0.005	0.115	0.003
175	6.40 * 10 ⁻⁸	600	20.1	0.9	5.7	0.3	2.2	0.1	0.110	0.003	0.123	0.002
180	1.10 * 10 ⁻⁷	660	20.0	0.4	5.6	0.2	2.1	0.1	0.105	0.002	0.138	0.001
165	6.23 * 10 ⁻⁸	600	20.3	0.6	5.6	0.2	2.2	0.1	0.106	0.002	0.141	0.002
160	4.21 * 10 ⁻⁸	600	18.9	0.8	5.3	0.2	1.9	0.1	0.102	0.003	0.141	0.002
155	3.24 * 10 ⁻⁸	600	20.4	1.0	5.8	0.3	2.2	0.1	0.107	0.004	0.143	0.003

Temp. (°C)	P _{cc} (mbar)	Time (s)	Ratio 1/18	Error 1/18	Size ¹ m/z=18	Error size 18	Ratio 1/75	Error 1/75	Ratio 45/30	Error 45/30
95	7.31 * 10 ⁻⁹	300	0.15	0.04	0.23	0.02	-	-	-	-
100	7.15 * 10 ⁻⁹	600	0.23	0.04	0.20	0.02	-	-	-	-
105	7.16 * 10 ⁻⁹	300	0.30	0.06	0.22	0.02	-	-	-	-
110	7.18 * 10 ⁻⁹	300	0.18	0.04	0.22	0.02	-	-	-	-
130	9.37 * 10 ⁻⁸	300	0.18	0.03	0.29	0.02	-	-	-	-
150	1.91 * 10 ⁻⁸	300	0.24	0.02	0.35	0.02	-	-	-	-
160 [†]	3.48 * 10 ⁻⁸	300	0.21	0.01	0.38	0.01	10	2	0.06	0.01
170	5.18 * 10 ⁻⁸	600	0.62	0.02	0.185	0.003	8.2	0.5	0.036	0.003
175	6.40 * 10 ⁻⁸	600	1.36	0.03	0.097	0.001	8.9	0.4	0.035	0.002
180	1.10 * 10 ⁻⁷	660	2.85	0.05	0.049	0.001	8.2	0.2	0.036	0.001
165	6.23 * 10 ⁻⁸	600	7.4	0.2	0.019	0.001	7.9	0.3	0.036	0.001
160	4.21 * 10 ⁻⁸	600	6.3	0.2	0.023	0.001	7.5	0.3	0.035	0.002
155	3.24 * 10 ⁻⁸	600	6.5	0.3	0.022	0.001	8.3	0.4	0.036	0.002

Table 3.2: Analysis of the measurement results.

¹ This the relative size, meaning the size divided by the total integral

[†] The peaks were very small and therefore the results are somewhat suspect, having large errors.

Due to a limited amount of available measuring time, measurements at temperatures where a lot of glycine had appeared were performed for a longer time than others. The only exception is at a temperature of 100 °C where a more detailed background picture was obtained.

Again it is clear that at a temperature of 150 °C, the molecule has started vaporizing. This can be seen from the glycine peak at m/z = 75, which starts appearing and increasing

from 150 °C. This peak was, however, too small to give meaningful ratios (see Fig. 3.4) and errors were very large.

It can also be seen that the ion pressure is related to the temperature. From a temperature of 150 °C the pressure constantly increases and decreases with temperature. This indicates that the glycine molecule starts to vaporizing from about $T = 150$ °C as well. At $T = 145$ °C there is also some vaporized glycine, as the first measurement showed.

In the absence of the molecule, both the peak at $m/z = 1$ and $m/z = 18$ can be regarded as background. The ratio between them shows no definite pattern when the temperature is below the evaporation temperature of the molecule, but it is also clear that there is no large change.

But once the molecule was evaporated, the ratio changed drastically. It can be seen that the peak size of $m/z = 18$ increases relative to the peak size at $m/z = 1$. This suggests that a fragment of $m/z = 18$ is formed once the molecule is present. This is due to NH_4^+ [10]. It must be noted, however, that the peak at $m/z = 1$ increases due to glycine fragments as well. This is not easy to see from this series of measurements. The relative size of the $m/z = 1$ peak decreases with temperature, but this is mainly due to the appearance of other glycine fragments.

A look at the coincidence analysis (see Fig 4.2) is much more insightful here, as it shows that hydrogen is a very common fragment. It can therefore be concluded that only a small amount of the measured hydrogen ions were from the background.

After the molecule was vaporized, the ratio between the peaks 30 and 75, 12 and 75, 28 and 75 and 12 and 30 was constant when one takes the statistical error into account.

However, because there was a limited available amount of measuring time, no more than five minutes could be waited in between measurements. The system did not have enough time to reach equilibrium, in the sense that the pressure was still changing slightly. The measurements itself were also too short.

When one compares the ion pressure at $T=160$ °C (first time) to the pressure at $T = 160$ °C (second time, see Fig. 3.4), a difference of about 20% can be seen. This shows how there was not enough relaxation time for the system, between subsequent measurements.

It is, however, good enough to see that the glycine molecule vaporizes around $T=150$ °C and that thermal dissociation does not happen at temperatures up to 180 °C.

This can be seen from the ratios of the peaks at $m/z = 75, 45, 30$ and 12.

Because the time between and during measurements was relatively short, the ratios changed until a temperature of temperature of 170 °C was reached.

It is expected that when the measurement time is increased, the ratios will be constant from temperatures of 150 °C. This will be tested during the next series of measurements.

The fact that the ratio between the peaks at $m/z = 75, 45, 30$ and 12 indicates that all of these are fragments from the molecule. Additionally, it shows that there is no thermal dissociation at temperatures up to 180 °C.

Other researches [9][10] conclude that the peak at $m/z = 30$ is the ion NH_2CH_2^+ , a fragment from the glycine molecule. The peak at $m/z = 28$ is also a fragment, being HCNH^+ . The peak at $m/z = 45$ is due to HOCO^+ , another large fragment.

During the next series of measurement, the same kind of experiment was done, but this time with a smaller temperature region and with longer measuring times. This led to the following results.

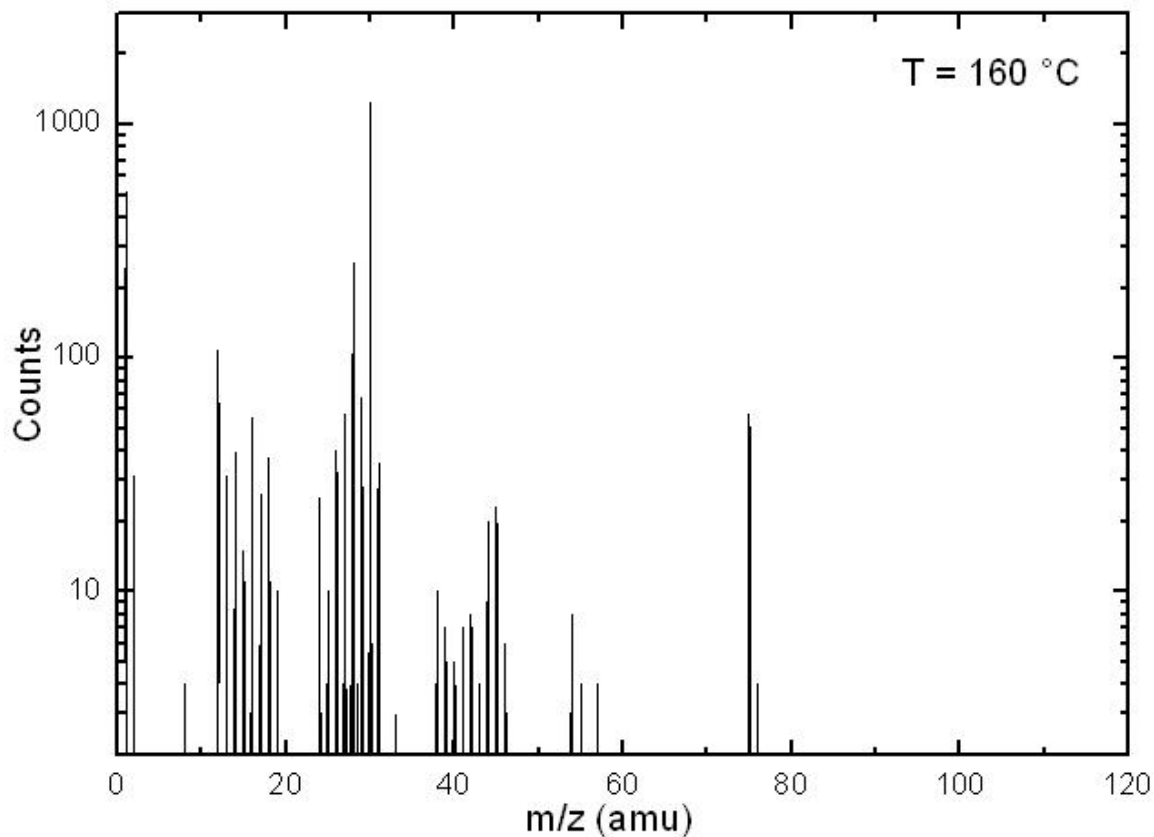


Fig. 3.3: Mass spectrum at $T=160\text{ }^\circ\text{C}$

T (°C)	P _{cc,initial} (mbar)	P _{cc,final} (mbar)	Rate _{initial} (s ⁻¹)	Rate _{final} (s ⁻¹)	size ¹ m/z=75	Error size 75	Ratio 28/75	Error 28/75	Ratio 30/75	Error 30/75
150	1.50*10 ⁻⁸	2.32*10 ⁻⁸	10	24	0.021	0.001	5.3	0.2	19.1	0.8
155	1.89*10 ⁻⁸	1.91*10 ⁻⁸	13	17	0.021	0.001	5.3	0.3	18.7	0.9
160	2.30*10 ⁻⁸	3.09*10 ⁻⁸	18	25	0.020	0.001	5.3	0.2	19.2	0.7
165	4.16*10 ⁻⁸	3.92*10 ⁻⁸	36	40	0.020	0.001	5.4	0.2	19.6	0.6

T (°C)	P _{cc,initial} (mbar)	P _{cc,final} (mbar)	Rate _{initial} (s ⁻¹)	Rate _{final} (s ⁻¹)	Ratio 45/75	Error 45/75	Ratio 45/30	Error 45/30	Ratio 18/75	Error 18/75
150	1.50*10 ⁻⁸	2.32*10 ⁻⁸	10	24	0.65	0.04	0.034	0.001	0.46	0.03
155	1.89*10 ⁻⁸	1.91*10 ⁻⁸	13	17	0.63	0.05	0.033	0.002	0.57	0.04
160	2.30*10 ⁻⁸	3.09*10 ⁻⁸	18	25	0.63	0.04	0.033	0.002	0.54	0.03
165	4.16*10 ⁻⁸	3.92*10 ⁻⁸	36	40	0.64	0.03	0.033	0.001	0.51	0.03

Table. 3.3: Measurements with increased time interval to reduce the error.

¹ The peak sizes have been divided by the total integral to obtain a better picture

In this measurement series, the statistical error was reduced, compared to the last measurement series. This lead to even smaller variations in the measured ratios.

It can be seen that the glycine molecule is already vaporizing at T = 150 °C.

At higher temperatures, the count rate is observed to be higher, while the ratios are still the same. This means that the molecule is not thermally being damaged.

Therefore, future measurements are recommended to be performed at temperatures of 165 °C up to 180 °C.

A comparison of glycine mass spectra from another research [5] is shown at the next page.

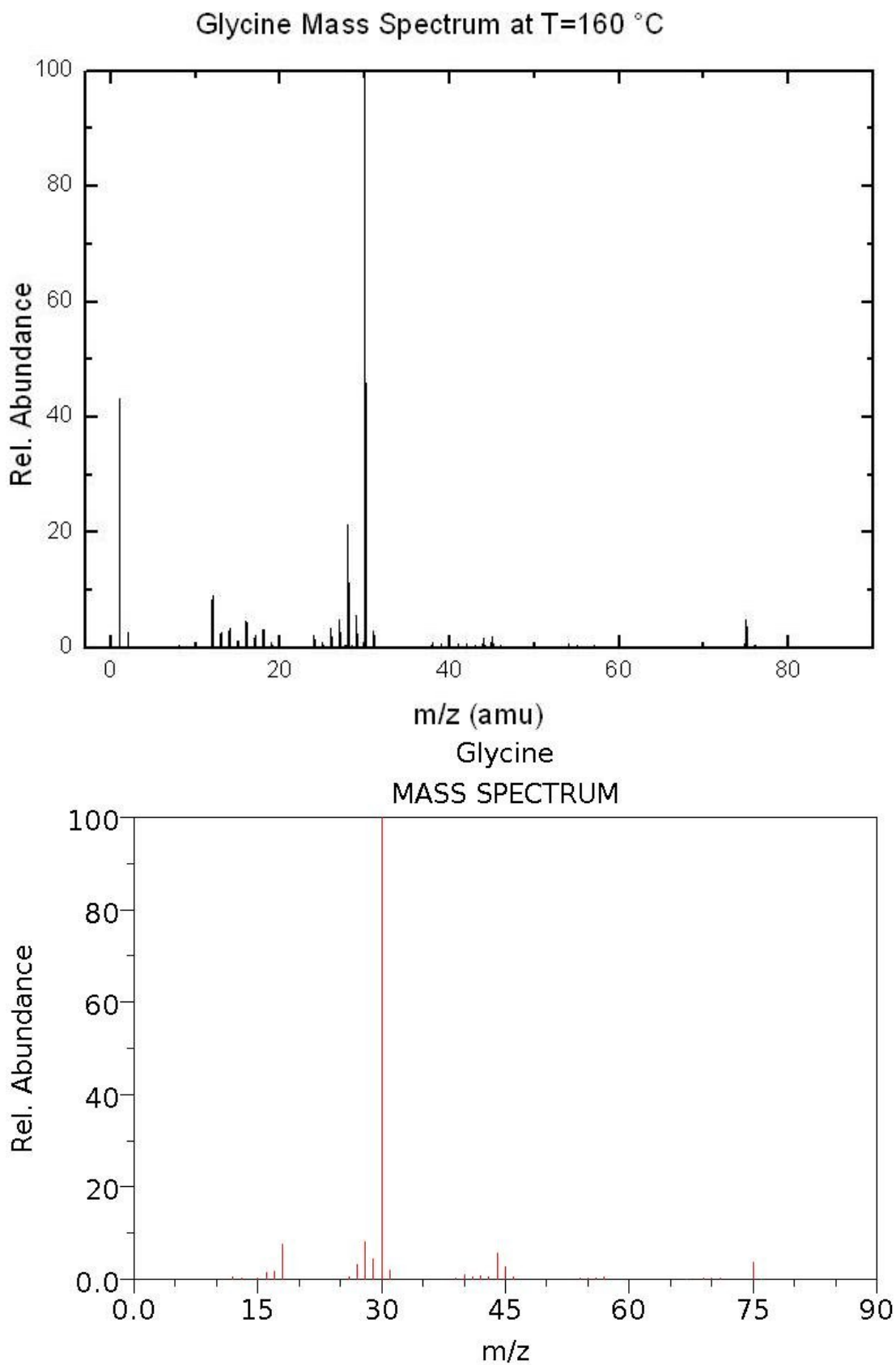


Fig. 3.4: Comparison of glycine mass spectra that we obtained (top) and one from NIST [5] (bottom).

The glycine spectra are very much alike and they share the same peaks. The only peak that is not there at the spectrum from NIST [5] is the hydrogen peak.

Coincidence measurement

In the coincidence measurement, various pairs of fragments can be identified.

The largest fragments are NH_2CH_2^+ ($m/z = 30$), HOCO^+ ($m/z = 45$) and HCNH^+ ($m/z = 28$). Other important fragments are NH_4^+ ($m/z = 18$, can be confused with water), H^+ ($m/z = 1$, can be confused with H^+ coming from water), O^+ ($m/z = 16$, can also be confused with O^+ from water), C^+ ($m/z = 12$) and N^+ ($m/z = 14$).

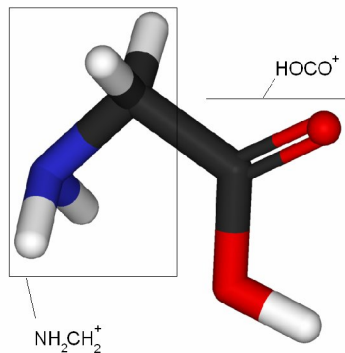


Fig 4.1: The glycine molecule. The two largest fragments are shown in the boxes.

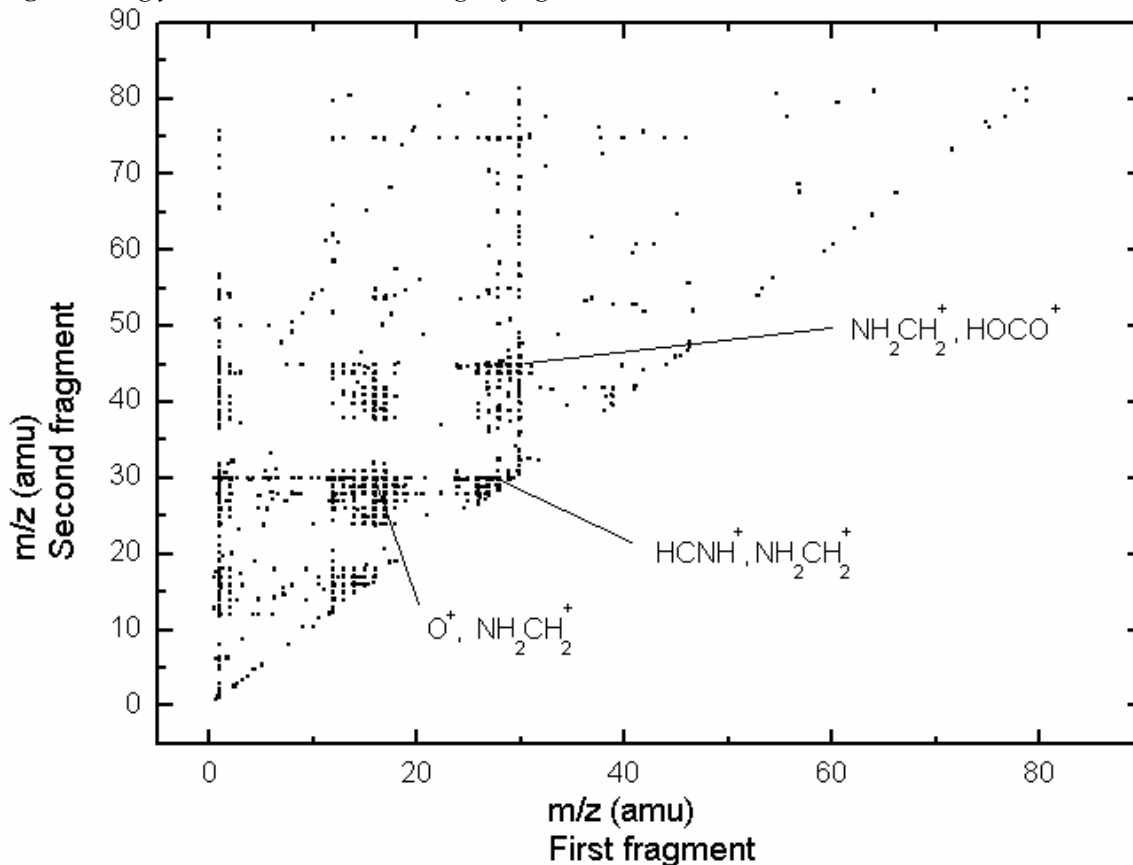


Fig 4.2: Coincidence graph. Several large islands are shown

When zoomed in on the islands, the following results are obtained.

Large fragments

Coincidence of the fragments HOCO^+ and NH_2CH_2^+ means a two body break up of the molecule. From Fig. 4.3 it can be seen that finding the fragments HOCO^+ and HCNH^+ together is more likely than finding a two-body breakup.

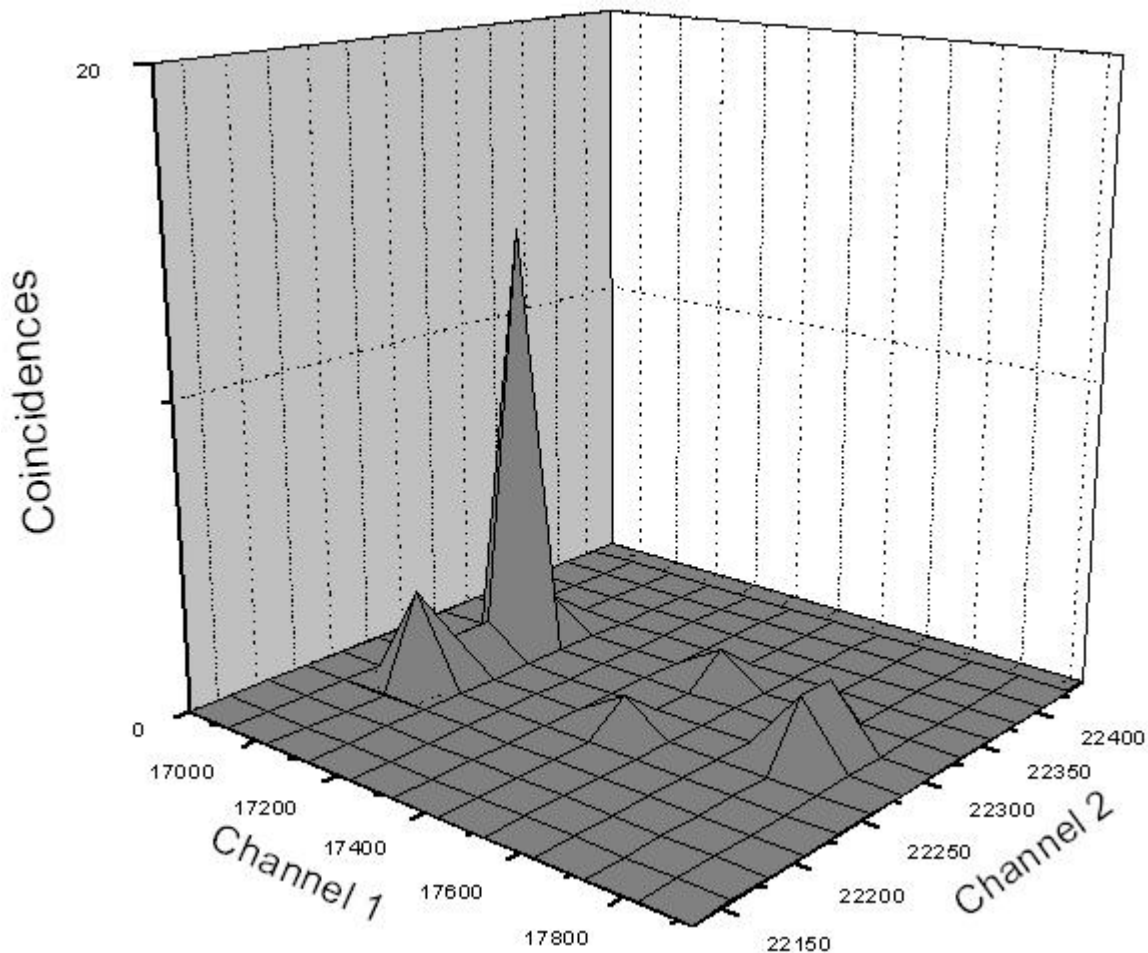


Fig 4.3: Graph of HOCO^+ ($m/z=45$) found in coincidence with NH_2CH_2^+ ($m/z=30$, the right peak) and HCNH^+ ($m/z=28$, the left peak).

Smaller fragments

Fig 4.4 shows various peaks of smaller fragments. These are carbon ($m/z=12$), CH^+ ($m/z=13$), nitrogen ($m/z=14$) and oxygen ($m/z=16$). The coincidence of CH^+ with carbon and nitrogen are less likely than coincidences of carbon with oxygen and nitrogen with oxygen. The largest island is coincidence of carbon with oxygen.

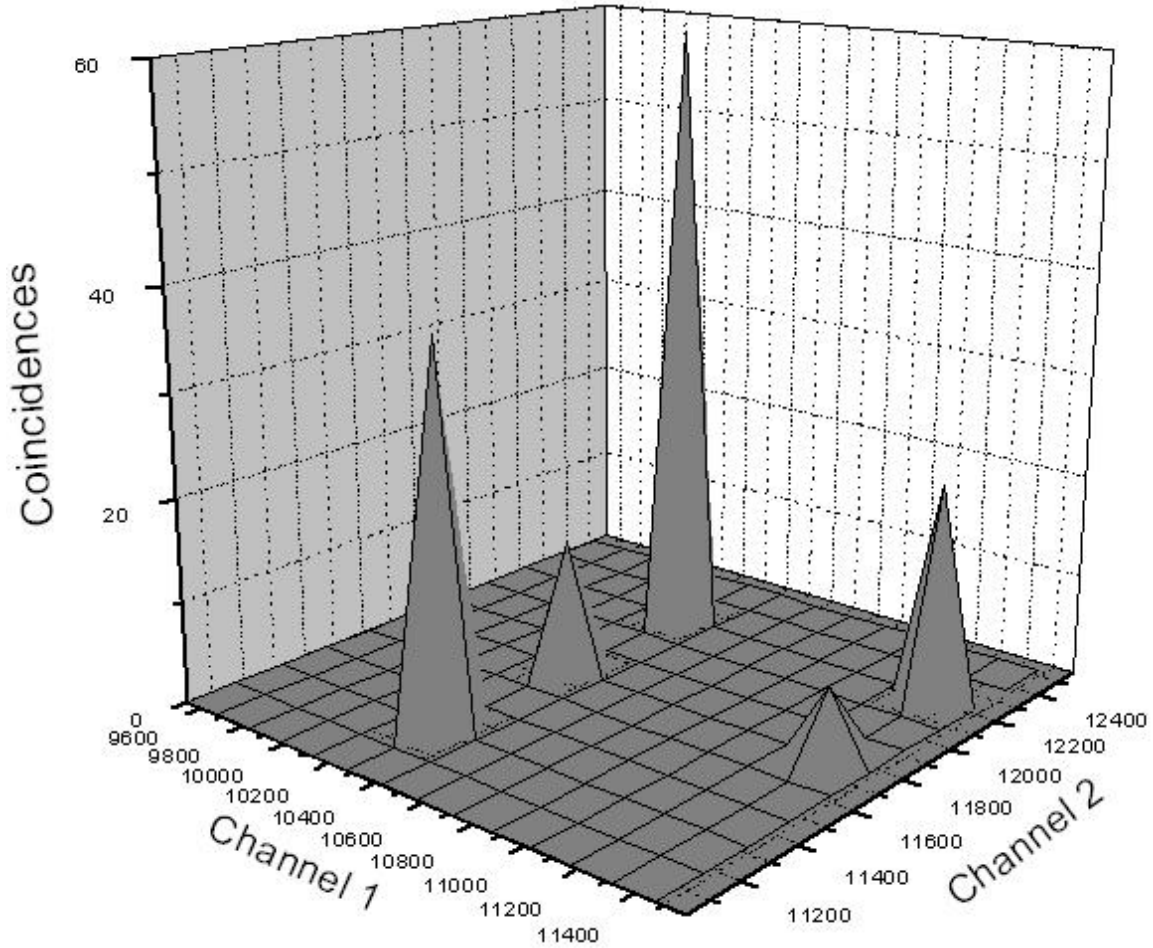


Fig 4.4: Coincidence graph, showing on the left carbon ($m/z=12$) and nitrogen ($m/z=14$). The peak in the middle is carbon and oxygen ($m/z=16$). The peak on the right side is nitrogen and oxygen in coincidence.

Kinetic energy calculation

Because the statistics are not sufficient, it is hard to separate the two different peaks for each island. Only at the coincidence of HCNH^+ ($m/z = 28$) and HOCO^+ , there was a clear separation of the two peaks.

The time difference between the two peaks makes it possible to make an estimation of the kinetic energy, by using formula (2.4).

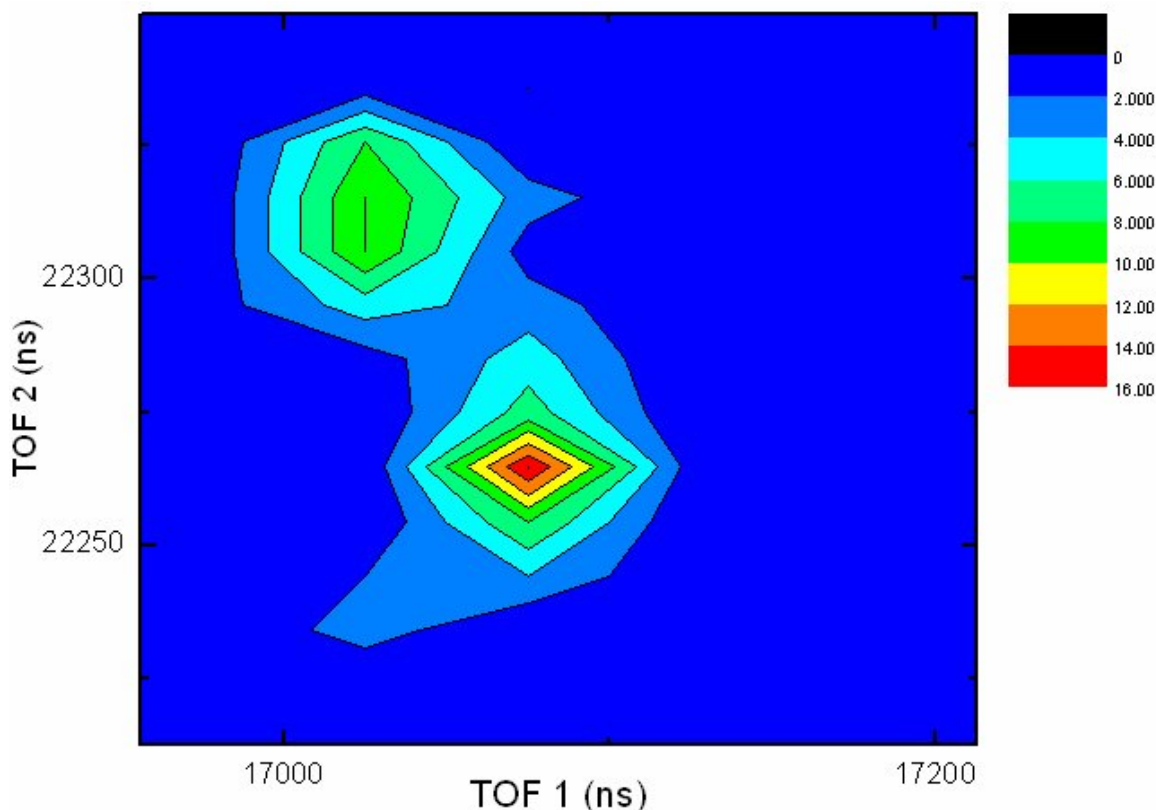


Fig 4.5: Contour plot of the coincidence island of HCNH^+ and HOCO^+ . Two different peaks in the island, Δt apart, can be seen.

$$U_{\text{ker}} = \frac{(\Delta t q E)^2}{8\mu} \quad (2.4)$$

Using SI units, we obtain:

$$\Delta t \approx 50 \text{ ns.}$$

$$q = 1.602 \cdot 10^{-19} \text{ C}$$

$$E = 600 \text{ V}$$

$$m_1 = 28 \text{ u} = 28 \cdot 1.66 \cdot 10^{-27} \text{ kg}$$

$$m_2 = 45 \text{ u} = 45 \cdot 1.66 \cdot 10^{-27} \text{ kg}$$

$$\mu = \frac{m_1 m_2}{m_1 + m_2} = \frac{28 \cdot 1.66 \cdot 10^{-27} \cdot 45 \cdot 1.66 \cdot 10^{-27}}{28 \cdot 1.66 \cdot 10^{-27} + 45 \cdot 1.66 \cdot 10^{-27}} = 2.87 \cdot 10^{-26} \text{ kg}$$

This gives:

$$U_{\text{ker}} = \frac{(\Delta tqE)^2}{8\mu} = \frac{(50 * 10^{-9} * 1.602 * 10^{-19} * 600)^2}{8 * 2.87 * 10^{-26}} = \frac{2.31 * 10^{-47}}{2.30 * 10^{-23}} = 1.00 * 10^{-24} \text{ J} = 6.3 \text{ } \mu\text{eV}$$

The value of 6.3 μeV is way too small, but i cannot find the wrong part in the calculation.

Summary

Fragmentation of the glycine molecule upon interaction of He^{2+} ions has been studied by using time-of-flight spectroscopy. Mass spectra show that the glycine molecule starts vaporizes at $T=145 \text{ }^\circ\text{C}$. Other studies found temperatures of $164 \text{ }^\circ\text{C}$ [9], $155 \text{ }^\circ\text{C}/165 \text{ }^\circ\text{C}$ [11] and temperatures between $150 \text{ }^\circ\text{C}$ and $200 \text{ }^\circ\text{C}$ [10]. Thermal dissociation was not the case even at temperatures as high as $180 \text{ }^\circ\text{C}$. Future measurements are recommended to be done at temperatures between $160 \text{ }^\circ\text{C}$ and $180 \text{ }^\circ\text{C}$, because at temperatures around $150 \text{ }^\circ\text{C}$ there is very little vaporized glycine which will result in a slower count rate.

During the coincidence measurement, several fragments were found in the islands, such as H^+ , C^+ , NH_4^+ , O^+ , HCNH^+ , CH_2NH_2^+ and HOCO^+ .

Although the statistics in the coincidence measurement were good enough to identify these islands, making an estimation for kinetic energy release (KER) turned out to be possible for only one island, and was $6.3 \text{ } \mu\text{eV}$.

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Uit introduction glycine:

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