Supporting File

Evaluating Air Quality through Ion Detection: An Application of JEOL Mass Spectrometry in Pollution Studies

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1. Theoretical Analysis

The spark ionization method is used to ionize the elements in the sample. This method is most widely utilized because it is most effective. Electrodes are made of the sample itself and a digital pulse of radio frequency (RF) is applied so that sparking takes place. The sample vaporizes and ionizes simultaneously in the ion source [1]. Ions are accelerated up to 30KV between the ion source and electrostatic analyzer. The accelerating potential determines the ion beam energy. This challenge has forced to development of more complex and versatile extraction electrode systems [2, 3]. To accelerate and focus the ions, a slit system is used in the spectrometer as shown in Figure S1.

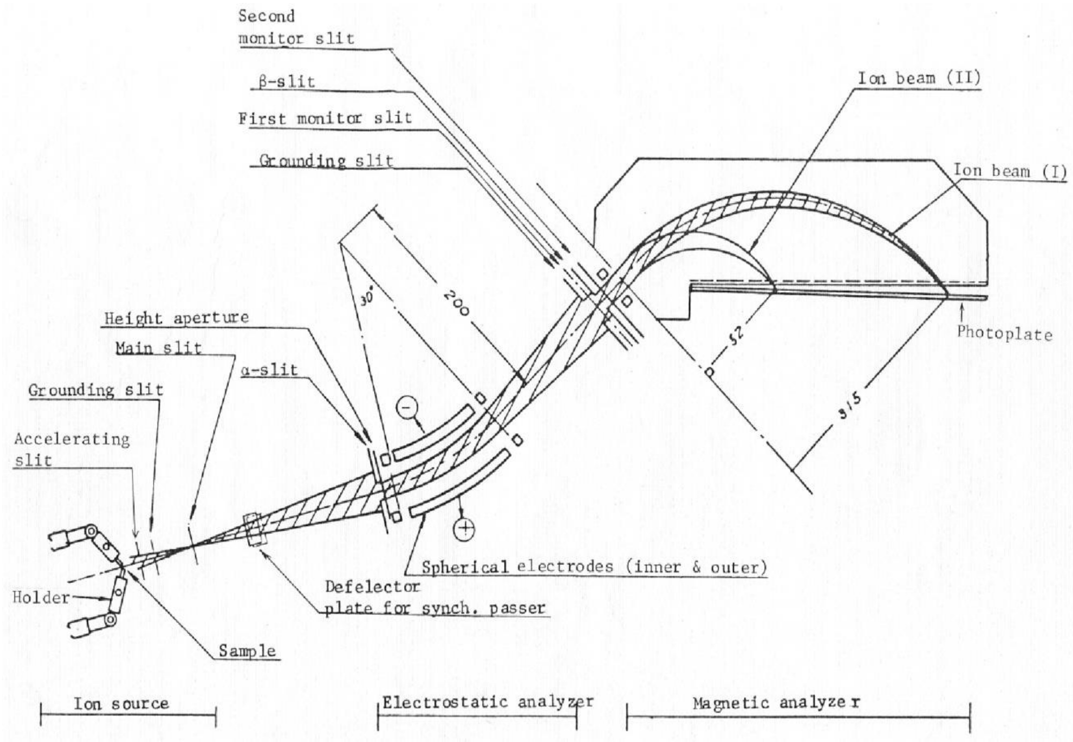


Figure S1: Schematic mass spectrometer with double focusing mechanism of the ion beam.

The ion beam passes through the electrostatic analyzer which gives the velocity focusing, an essential requirement to separate the ions purely on the m/e basis in the magnetic analyzer. The kinetic energy gained by the ion is as given below,

$$K.E. = \frac{mv^2}{2} = qV.........1$$

Where m is the mass of the ion with charge q and accelerated through a voltage *V*. After passing through the electrostatic analyzer, ions move into a magnetic analyzer where the uniform magnetic field H is perpendicular to the direction of ions and ions will follow a circular path of radius R due to the Lorentz force.

$$F = qvH = \frac{mv^2}{R} ....2$$

In the electrical detection system, the ions enter with a constant velocity, due to the electrostatic analyzer, the magnetic field is scanned and peak spectra are detected in the form of an electrical signal at a fixed radius position as shown in Figure S2.

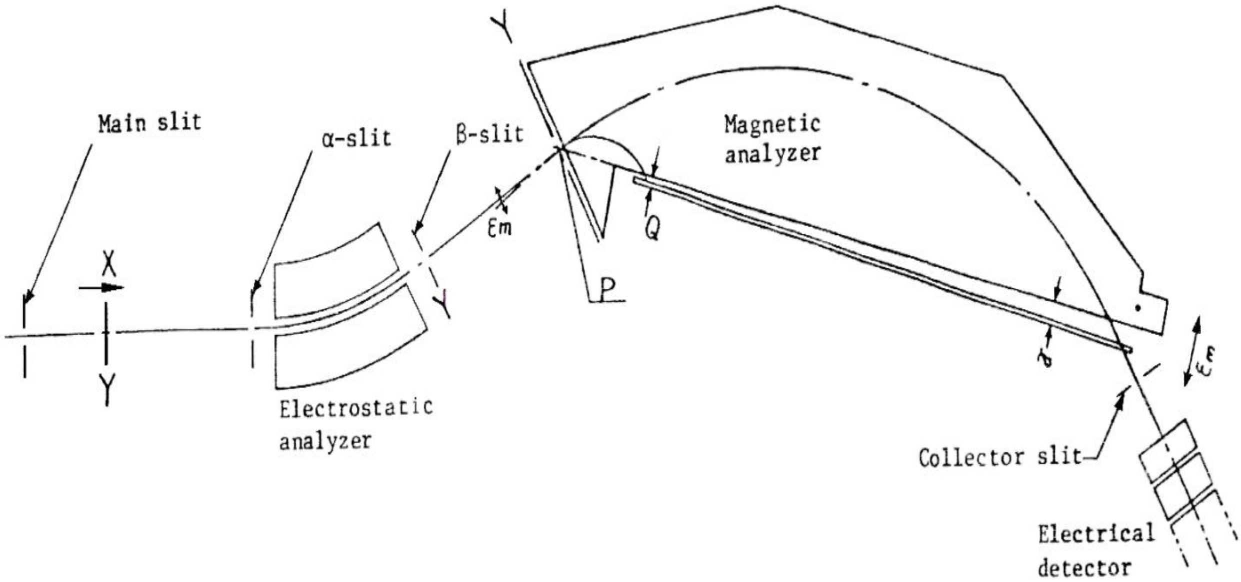


Figure S2: Ion detection mechanism at collector slit in the Electrical detection system (EDS).

$$\frac{m}{q} \propto H ....3$$

Since the direction and velocity of the ions differ according to the stage of ionization, focusing is difficult even though the ions possess an identical m/q. In order to separate and focus the ions in a uniform magnetic field on the bases of m/q the ions must have the same velocity. As the ions pass through the circular electric sector they are under the influence of circular electric field E which provides the centripetal force.

$$\mathrm{F} = q\frac{\mathrm{V_e}}{\mathrm{L}} = \frac{\mathrm{mv}^2}{\mathrm{r}} ....4$$

Where r is a radial path of ions passing through the cylinder electrodes of the electric sector having voltage V_e and L is the separation between these cylinder electrodes.

The outer cylinder is at a positive potential with respect to the inner cylinder as shown in Figure 1. A radial electrostatic field is set up between the two cylinders.

Rearranging the above equation

$$\frac{\frac{1}{2}mv^2}{q} = \frac{\mathrm{rV_e}}{\mathrm{2L}} \text{..........5}$$

Or

$$\frac{K:E}{q} = \frac{\mathrm{rV_e}}{\mathrm{2L}} \text{..........6}$$

A cylindrical electric sector disperses ions according to their Kinetic charge ratio. It is used as a velocity-focusing element.

From equation 4

$$\frac{m}{q} = \frac{rV_e}{v^2 L} \text{..........7}$$

So the ions of the same element with the same charge will exit from the electric sector with constant velocity v. JEOL used Mattauch-Herzog technique [4] to separate the ions purely on the m/q basis. In this technique, the electrostatic field is used in conjunction with the magnetic field to focus the velocity and direction. The particular advantage of this method is that separated ions are focused on a single focal plane at the exit boundary of the magnetic field. Mattauch & Herzog instrument [5] was completed in Vienna in 1935. It possesses a double focus for all masses. It is designed such that a (31.82°) electric sector, a drift length which is followed by a (90°) magnetic sector.

A radial electrostatic field is set up between the two spherical electrodes and the potential along the central path is zero [6]. The ion beam will have a rotating radius of 200mm if the relation between the electrostatic field voltage V_e and the accelerating voltage V is established by the formula $V_e = V/10$.

The JMS-01BM-2 consists of an ion source, analyzer system, ion detection system (Photo plate & Electrical) and vacuum system. A block diagram of the basic components of JMS-01BM-2 is shown in Figure S3 [4]. The ion detection system can be used for ion implantation.

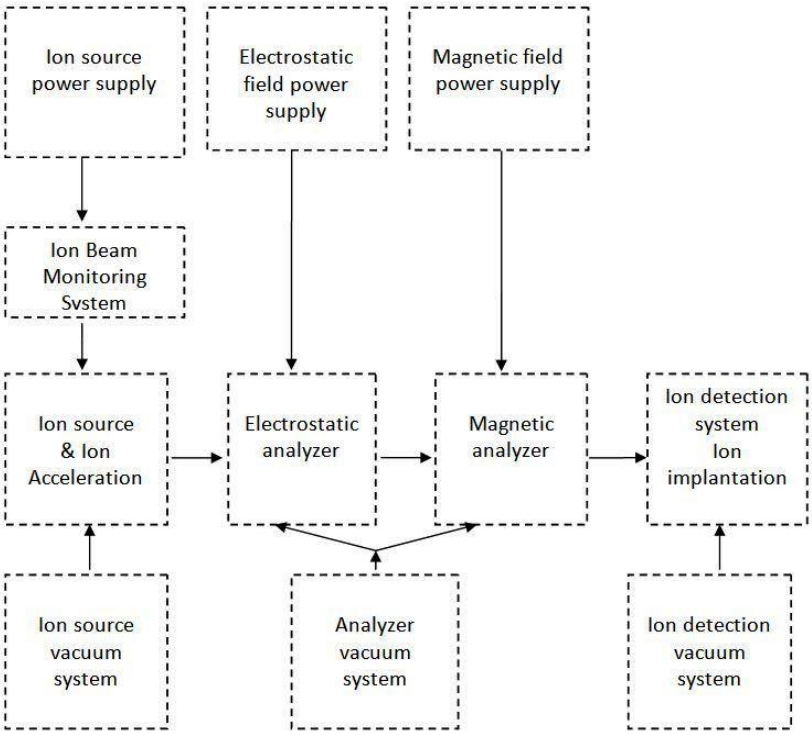


Figure S3: Basic construction of JMS-01BM-2.

The electrical detection system was used for mass analysis. The analysis chart is shown in the Figure S4.

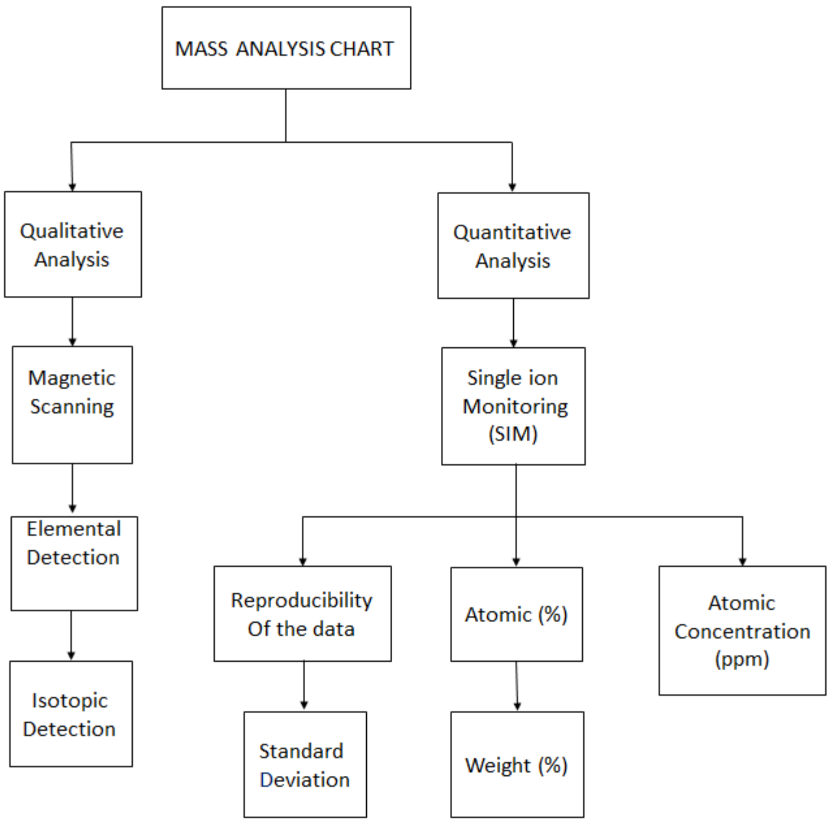


Figure S4: Mass analysis chart.

For the qualitative analysis of the sample, the magnetic field was scanned between two preset values as programmed in the EDS. It gives the details of the constituent elements in the sample. The ratio of the elemental ion beam to the total ion beam was plotted. Therefore, the variation in the ion beam due to the variations in the ion production was minimized. For any detected element at the collector slit the corresponding peak on the chart was obtained. The magnetic field values of the peaks were measured from the chart. For each peak, the corresponding atomic mass was calculated using the formula.

$$M = \frac{A_m^2 H^2}{VK^2} \text{..........8}$$

Where A_m is the rotating radius in electrical detection mode = 30.74cm, K is constant = 143.6, V is Accelerating voltage = 25000 V, H is magnetic field intensity (Guess), measured from the graph of qualitative analysis, M is the atomic mass of detected ion (a.m.u). To find out the elements for corresponding mass numbers data book was used [7, 8].

For the quantitative analysis of the sample, EDS was used in the peak switching mode. The elements were detected from the peak spectra. These elements were labelled and their corresponding magnetic field (H) values were noted. The magnetic field values of the detected elements were loaded on channels of the EDS panel. In the peak switching mode, the ion detectors were used in the charge collection mode. These charges were indicated on the electrometers of the EDS panel. The maximum amount of charge to be accumulated from the total ion beam can be set on the EDS panel for a single reading.

The total ion magnitude (TIM) was measured on the detector at the entrance of the magnetic field and the detected ion magnitude (DIM) of the detected element was measured on the detector at the exit of the magnetic field. To get the actual result, background values were subtracted from the corresponding TIM and IM values. The accumulated charge of each TIM and IM value was then multiplied with the corresponding multiplicity factor. The ion range had final TIM and IM values. To achieve more accurate and better results, four sets of such readings were taken. These quantities were printed on the digital printer as shown in the chart in Figure S5. The data of these sets was used for the quantitative analysis. The complete quantitative analysis gives the details of atomic percentage, weight percentage and other statistical information [9].

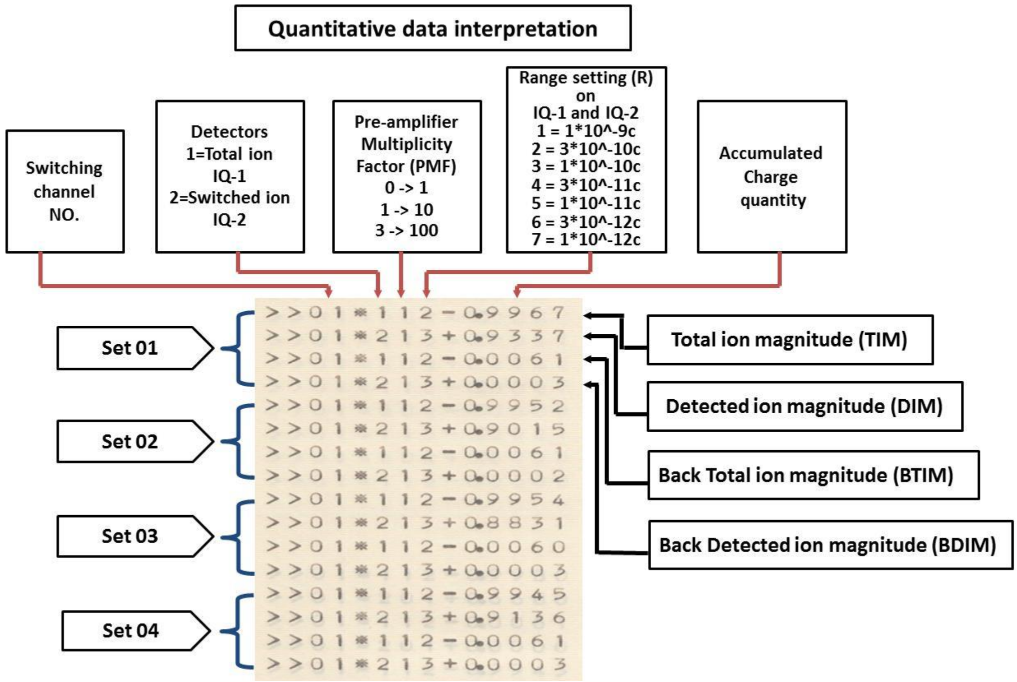


Figure S5: Quantitative analysis data chart.

The ratio of elemental ion to the total ion is calculated by the formula given below;

$$X_i = \frac{[\mathrm{DIM} - \mathrm{BDIM}] \times \mathrm{PMF} \times \mathrm{R}}{[\mathrm{TIM} - \mathrm{BTIM}] \times \mathrm{PMF} \times \mathrm{R}} \quad ....9$$

The average value of sets is measured by the formula given below.

$$\overline{X} = \frac{\sum_{i=1} X_i}{n} \quad ....10$$

The atomic percentage of an element from all the detected elements is calculated by the formula given below;

$$\text{Atomic } \% \text{ age} = \frac{\overline{X}_i}{\sum_{i=1}^{n} \overline{X}_i} \times 100 \quad ....11$$

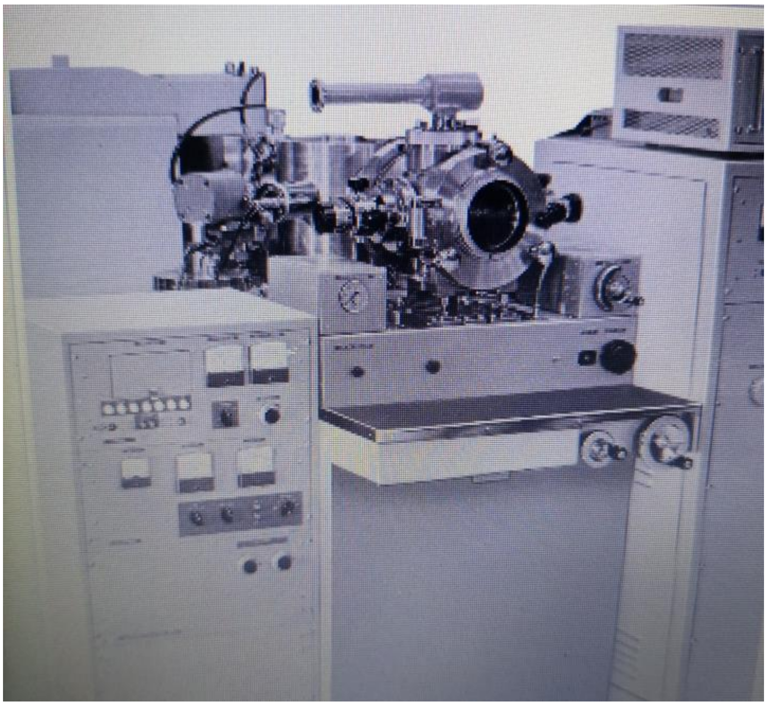
The weight percentage is calculated by the formula given below;

$$\text{Weight } \% \text{ age} = \frac{Y_i}{\sum_{i=1}^{n} Y_i} \times 100 \quad ....11$$

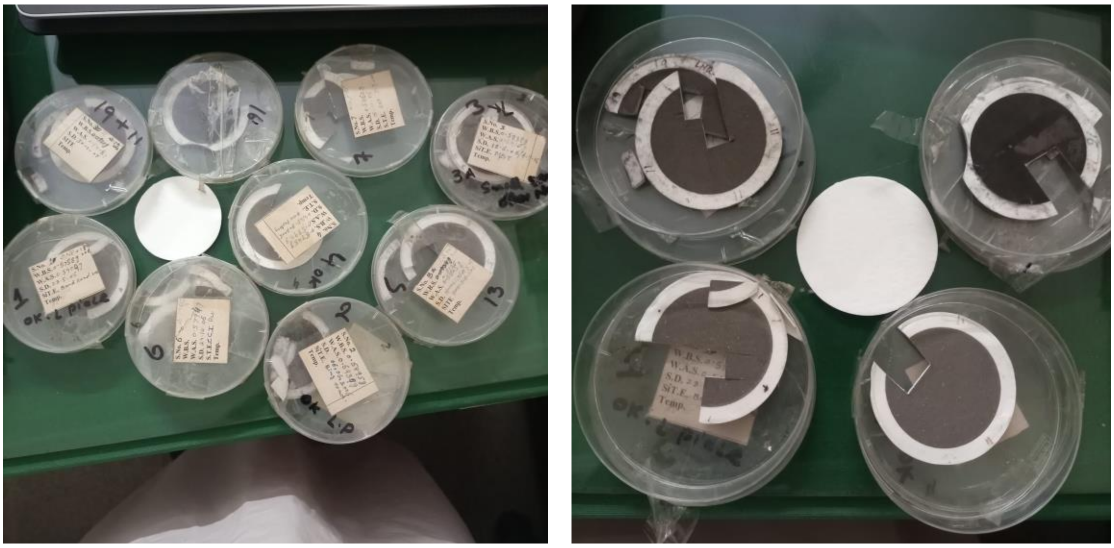
Where Y is equal to the atomic percentage multiplied by the detected mass. In the qualitative analysis graph, the magnetic field values were measured with the help of

Auto CAD for better accuracy. The qualitative and the quantitative analyses were performed in MS Excel to minimize the errors for all the calculations.

2. Prepared Samples



(Jeol Mass Spectrometer)



(Prepared Samples for characterization)

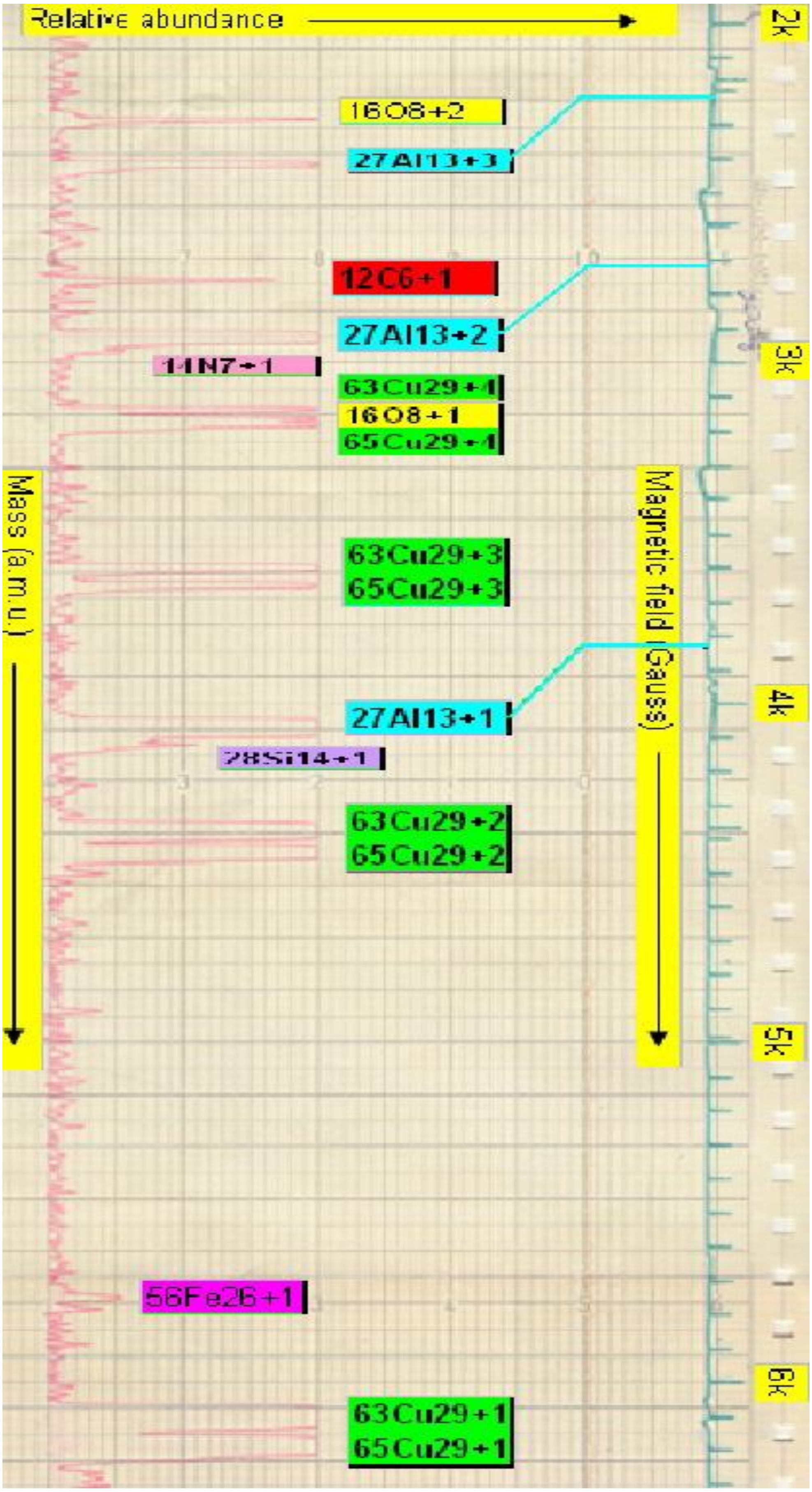


Figure S6: Elements detected in Aluminum-Copper sample

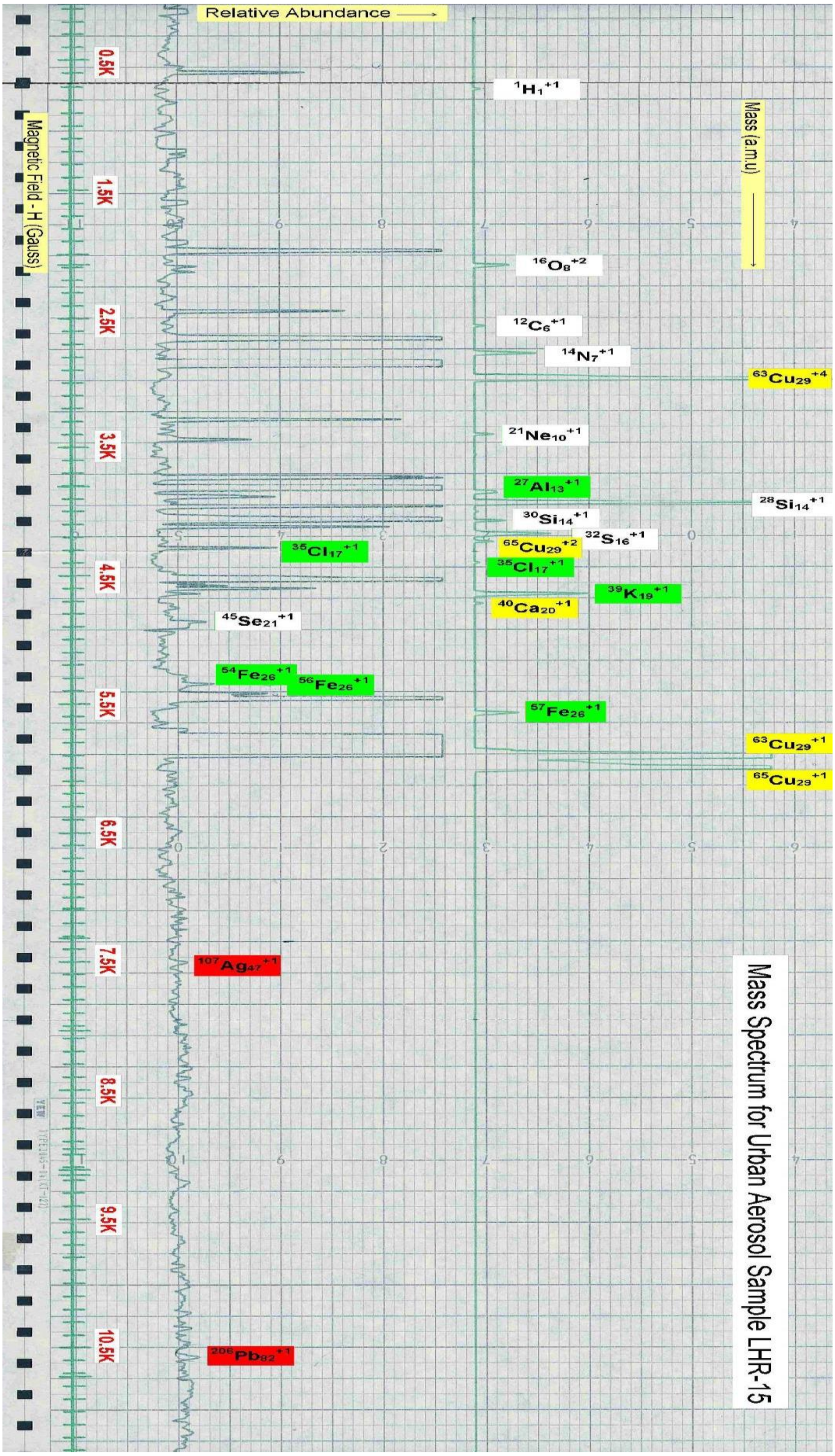
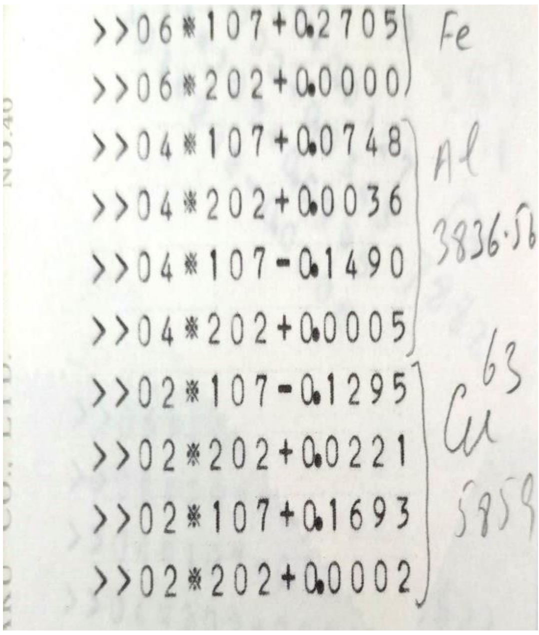


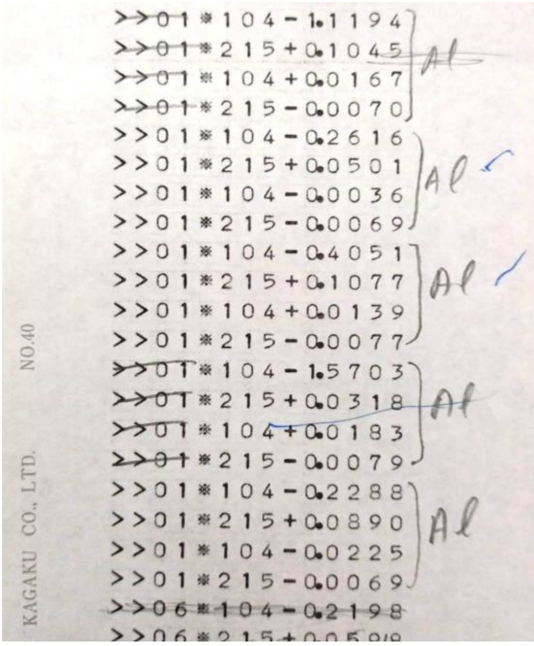
Figure S7: Elements detected in the aerosol sample

3. System Generated Results

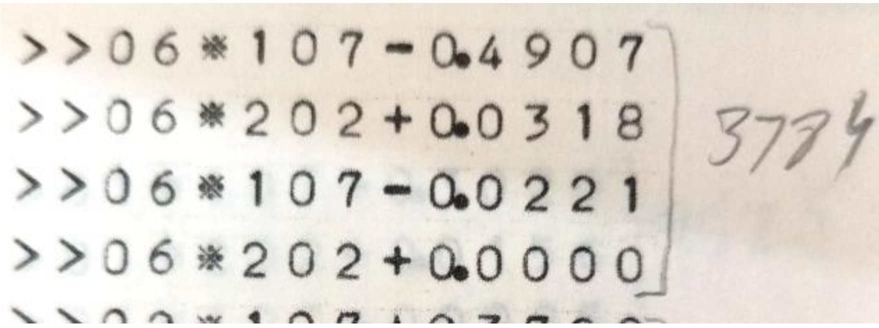
- **Data Form Output**



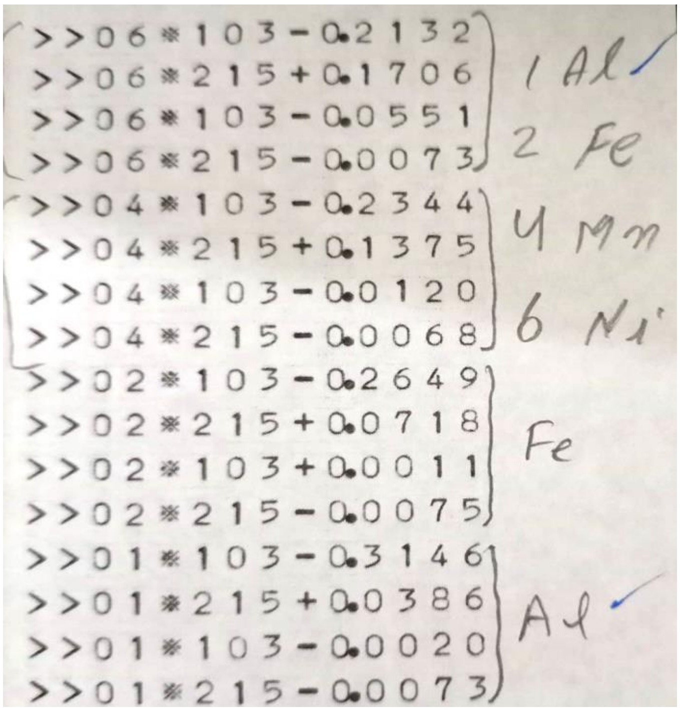
>>06*107+0.2705
>>06*202+0.0000
>>04*107+0.0748
>>04*202+0.0036
>>04*107-0.1490
>>04*202+0.0005
>>02*107-0.1295
>>02*202+0.0221
>>02*107+0.1693
>>02*202+0.0002



>>01*104-1.1194
>>01*215+0.1045
>>01*104+0.0167
>>01*215-0.0070
>>01*104-0.2616
>>01*215+0.0501
>>01*104-0.0036
>>01*215-0.0069
>>01*104-0.4051
>>01*215+0.1077
>>01*104+0.0139
>>01*215-0.0077
>>01*104-1.5703
>>01*215+0.0318
>>01*104+0.0183
>>01*215-0.0079
>>01*104-0.2288
>>01*215+0.0890
>>01*104-0.0225
>>01*215-0.0069
>>06*104-0.2198

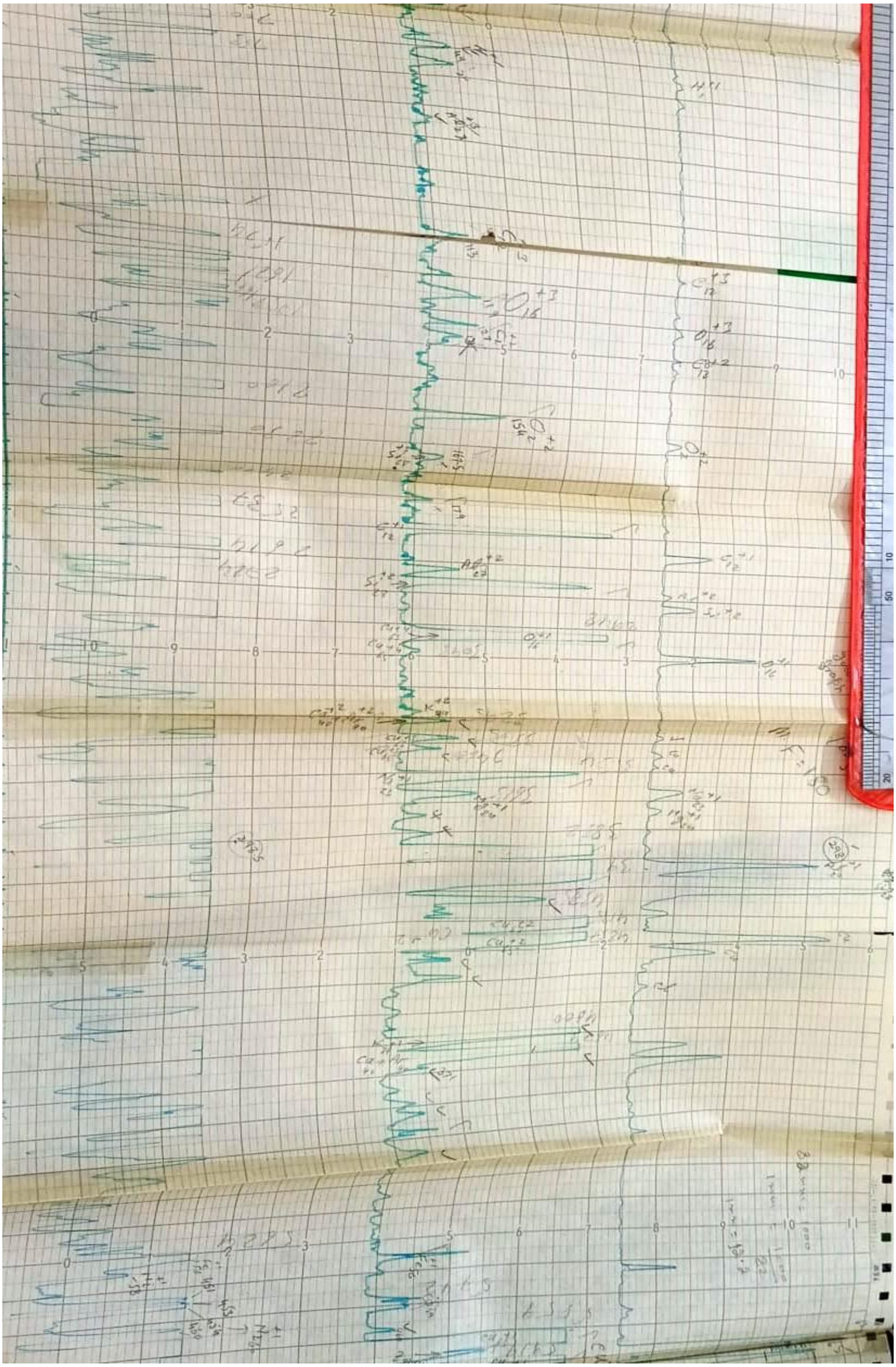


>>06*107-0.4907
>>06*202+0.0318
>>06*107-0.0221
>>06*202+0.0000



>>06*103-0.2132
>>06*215+0.1706
>>06*103-0.0551
>>06*215-0.0073
>>04*103-0.2344
>>04*215+0.1375
>>04*103-0.0120
>>04*215-0.0068
>>02*103-0.2649
>>02*215+0.0718
>>02*103+0.0011
>>02*215-0.0075
>>01*103-0.3146
>>01*215+0.0386
>>01*103-0.0020
>>01*215-0.0073

- **Graph Form Output**



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