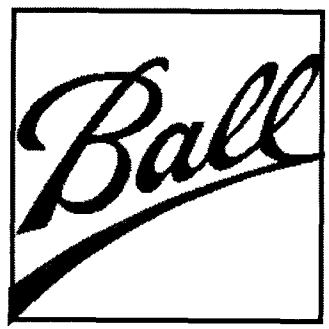
# Miniature Electrospray Ionization/Ion Mobility Spectrometer (ESI/IMS) System for Detection of Organic Molecules on Mars


National Aeronautics and
Space Administration
Jet Propulsion Laboratory
California Institute of Technology



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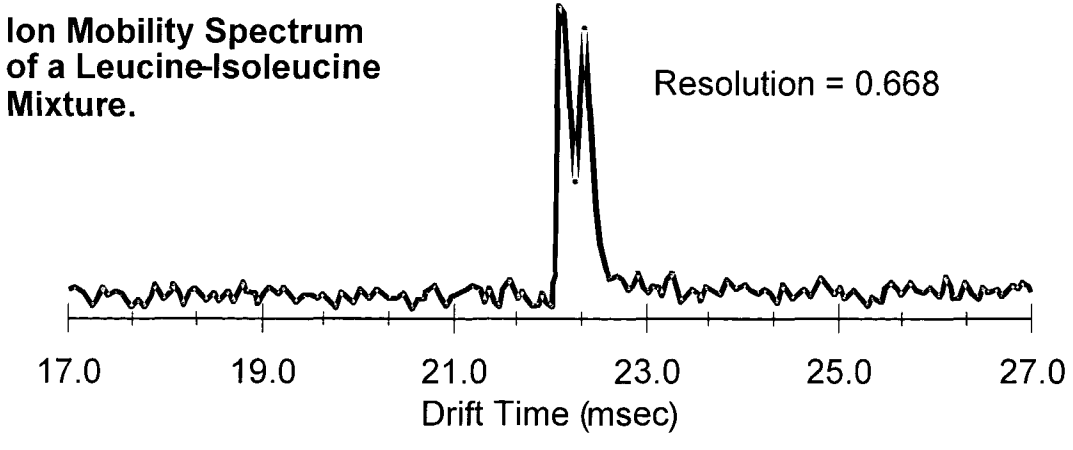
# Electrospray Ionization/Ion Mobility Spectrometry (ESI/IMS)

- Electrospray ionization (ESI) and high-resolution ion mobility spectrometry (IMS) have been incorporated to detect biologically relevant compounds in complex matrices.
- ESI is a soft ionization method in which molecules can be ionized at elevated pressures. This makes it a natural choice for incorporation with ion mobility spectroscopy, which also operates at elevated pressures. IMS is simple, fast, rugged, highly selective and very sensitive to a wide range of compounds.
- Selectivity and separation by IMS are functions of ion size and mass, rather than being dependent on mass only, as in mass spectrometry.




An ion mobility spectrum of a Leucine/Isoleucine mixture which demonstrates IMS's ability to separate isomers (obtained by the JPL team in collaboration with Washington State University using a high-resolution IMS).

## Advantages of ESI/IMS:

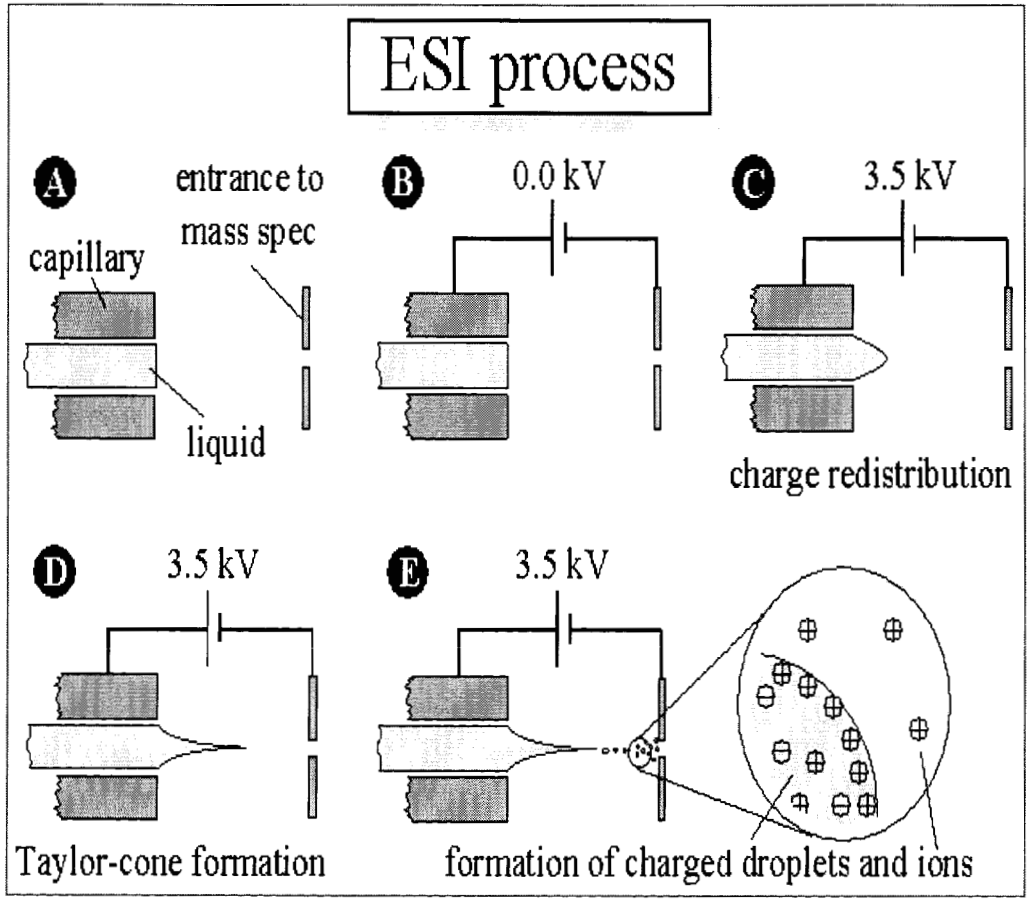
- Simple and inexpensive to construct
- Fast (samples can be run in less than a minute)
- Rugged construction (no moving parts, can take large g forces)
- Highly selective
- Very sensitive (parts per billion)
- Unlimited mass range
- Able to operate at wide pressure ranges (~ 1 to 760 Torr)
- ESI/IMS is completely self calibrating.

## Advantages over Gas Chromatography (GC):

- ESI/IMS is capable of analyzing high refractory compounds.
- Ion mobility constants provided by IMS contain more information (mass/size/structure) than GC retention times.
- Analysis times for IMS are at least 3 orders of magnitude faster than GC

# Electrospray Ionization (ESI):

The advantage of ESI in the analysis of biologically important molecules stems from the fact that ESI is able to extract these fragile chemical species from solution intact, ionize them, and transfer them into the gas phase where they can undergo analysis by a spectrometer. ESI allows one to detect very large biological compounds, ones with masses up to several million amu, including proteins and DNA.



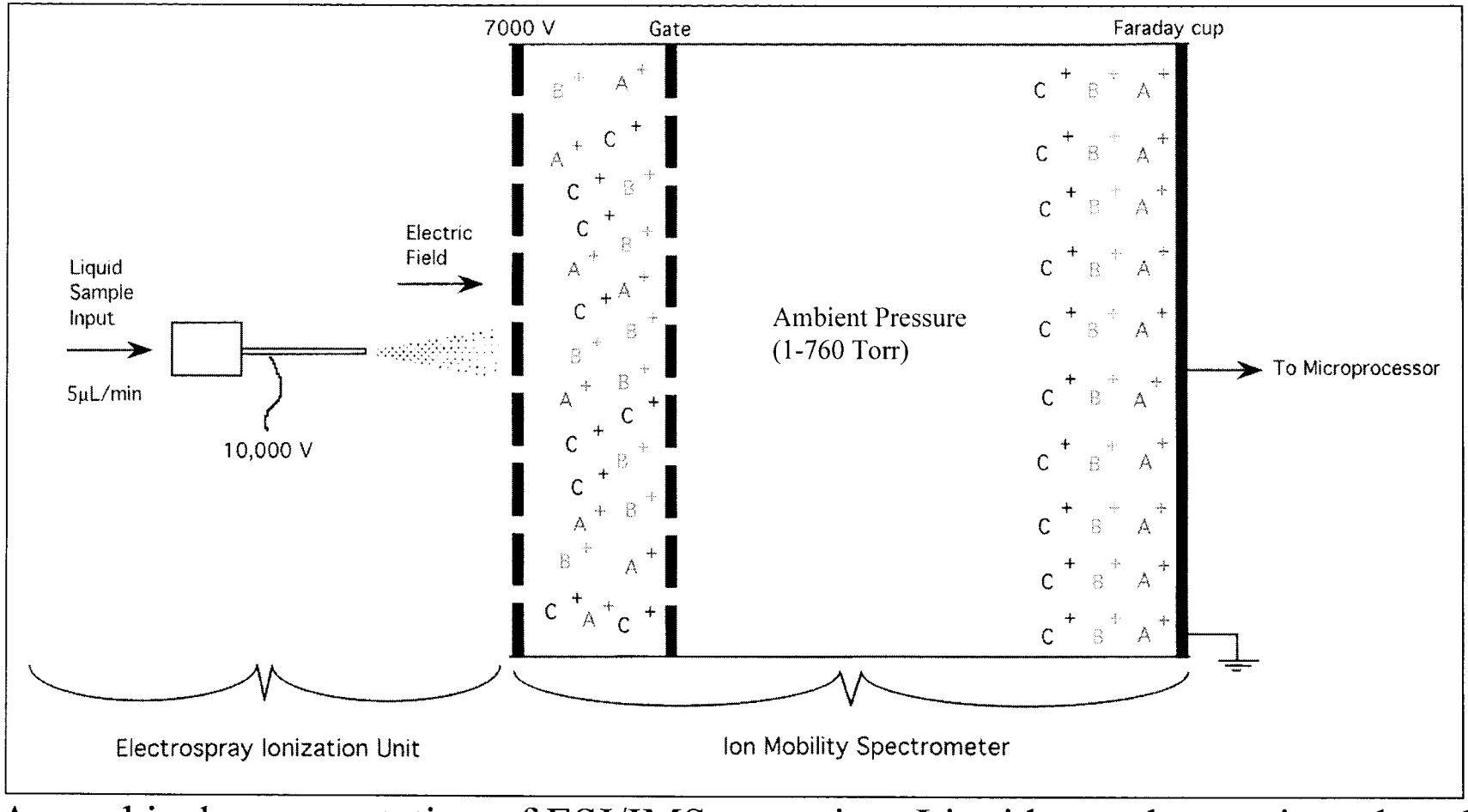
# Ion Mobility Spectrometry (IMS)

**Concept:** Ions are separated by their "gas phase mobilities" as they travel through a neutral drift gas under the influence of an electric field. As ions migrate in the direction of the field, they suffer many collisions with neutral molecules. Over macroscopic distances, this results in a constant average ion velocity, which is dependent on the electric field as well as the ion-molecule collision cross sections. By recording the drift time of an ion through a fixed distance, its "mobility", $K_0$, can be determined and used to identify the parent molecule.

$K_O=(L/t_d\ E)(P/760)(273/T)$

$t_d$ is the ion drift time
E is the electric field strength
L is the length of the drift tube
P is the buffer gas pressure
T is the normalized buffer gas temperature

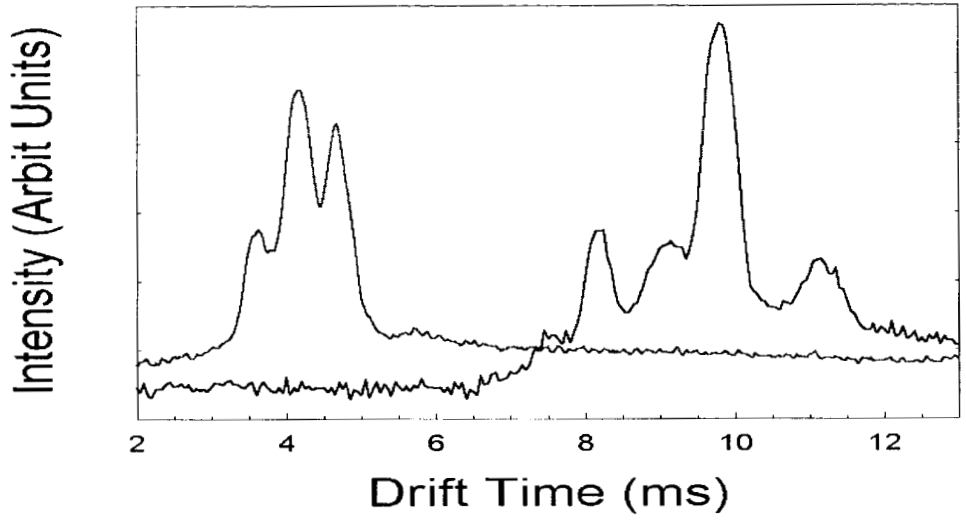
**Instrument:** Ion mobility instruments consist of an ionization source and a drift tube. The drift tube is often formed by a stack of ring electrodes at potentials, which produce a linear potential gradient along the axial direction. An ion gate allows ion pulses to enter the drift region and migrate toward an electrometer. Recording the ion current as a function of drift time produces an IMS spectra.



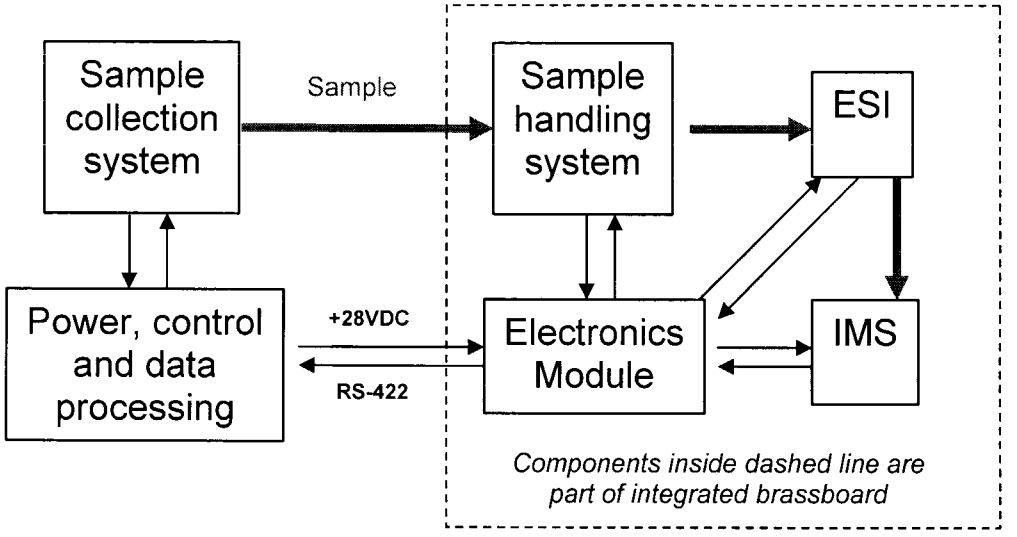

A graphical representation of ESI/IMS operation. Liquid samples are introduced by a needle which is held at a fixed potential above a grid. Ions are formed as the liquid droplets dissolve in a region between the grid and the gate. The Gate is pulsed at regular intervals and the ions separate as they migrate in the electric field of the drift region. All of these regions are at ambient pressures.

# Key Features of the Breadboard IMS Design

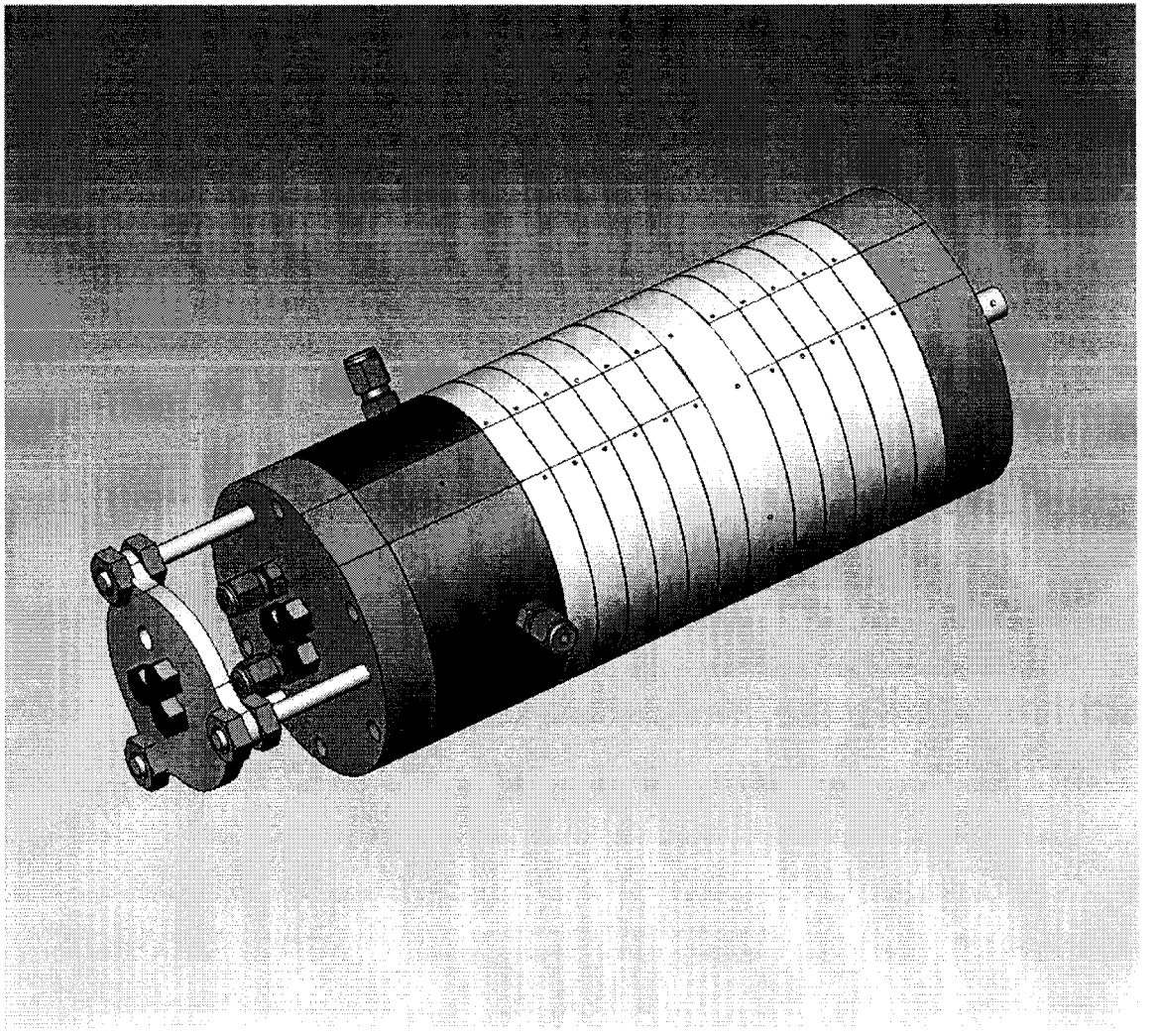
- The IMS instrument developed for this project is completely portable.
- The instrument is isolated from the environment.
- The instrument can operate at pressures between 1-760 Torr.
- The design is modular. This allows for experimental optimization of both the desolvation and drift tube lengths.
- A recyclable drift gas system has been and incorporated into the design in order to minimize the amount of expendable material required by the instrument.
- The ESI source was designed with multiple capillaries. This allows for simple switching of sample liquids and provides redundancy to ensure reliable field operation.



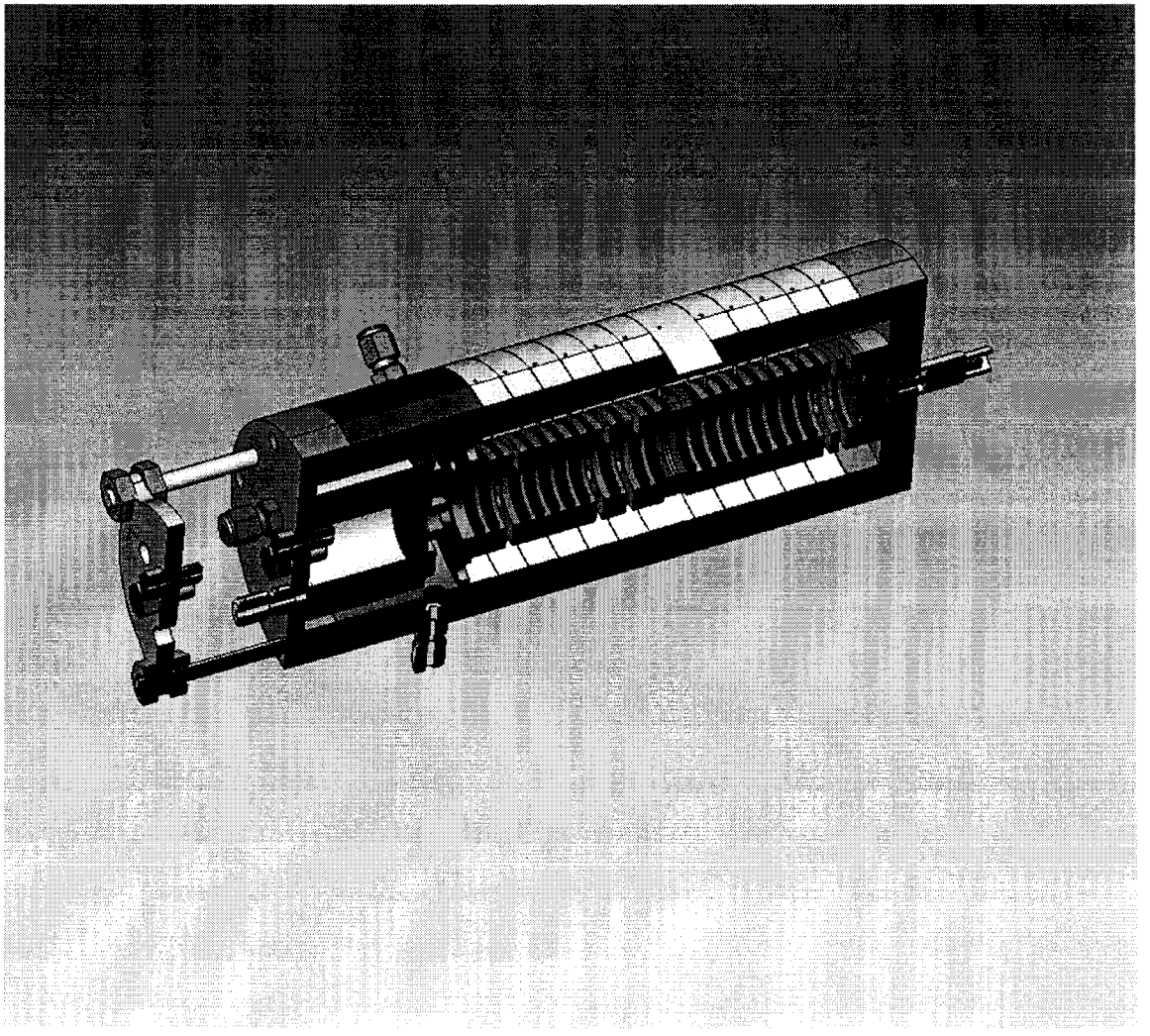

Ion Mobility spectra of a Methanol/Acetic Acid/Water solvent mixture at 30 Torr (red) and at 760 Torr (blue). At 30-Torr, the ESI needle was at 1900 V with respect to the Faraday cup with 770 V over the drift cell. At Martian pressures (~5 Torr), we expect a drift voltage of ~200 V.




**Functional block diagram of stand-alone brassboard test system**



CAD drawing of the ESI/IMS instrument (isometric view).



CAD drawing of the ESI/IMS instrument (isometric view-cross section).

Acknowledgment: The research described in this poster was performed at the Jet Propulsion Laboratory, California Institute of Technology and at Ball Aerospace & Technologies Corp. The research was supported by NASA's Mars Instrument Development Program.

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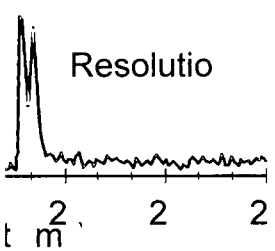


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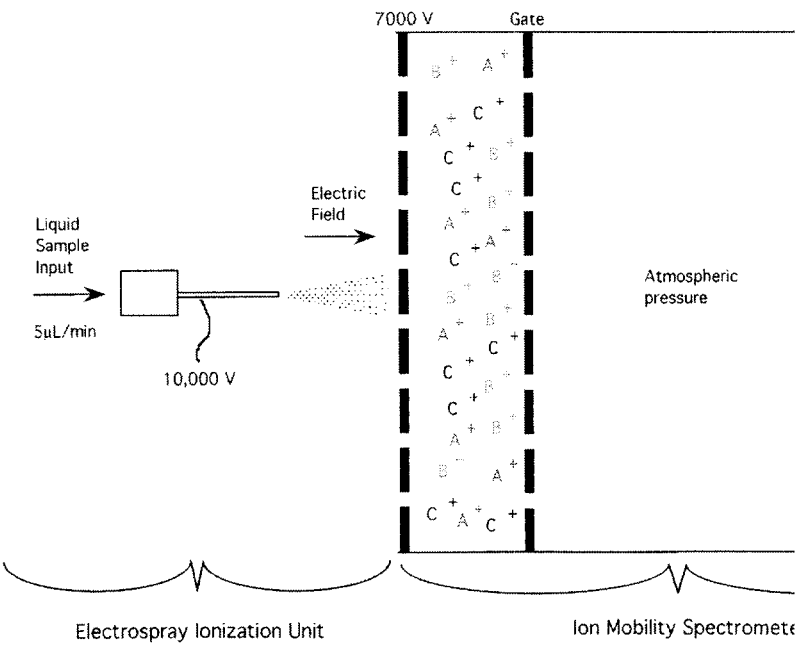


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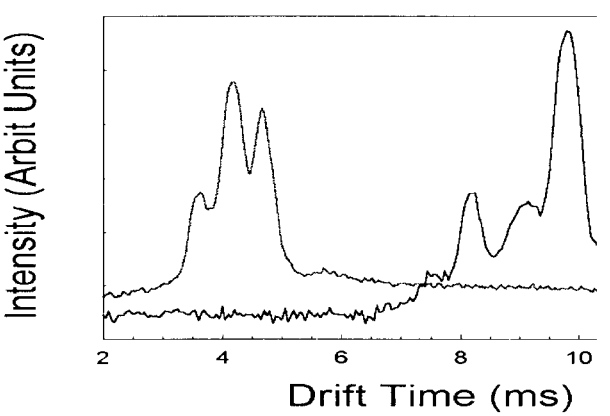


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