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Hardware Article

Implementation of a flexible, open-source platform for ion mobility spectrometry

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ABSTRACT

When operated as a stand-alone device, an ion mobility spectrometer (IMS) routinely offers low limits of detection (pptv-range) for gas-phase analytes even for measurement times less than a second. Mass analyzers further enhance the analytical power of IMS separations, however, high performance drift-cell IMS instruments are often highly customized, relatively large, and require extensive expertise to operate. In this work we present an optimized, low cost IMS system that leverages an easy-to-assemble ion gating structure that enables IMS spectra with resolving powers exceeding 90 for a drift cell only 10 cm in length. The IMS presented in this work consists of stacked rings divided by spacers all fabricated from printed circuit boards (PCB). The rings are connected via a slotted PCB-board containing a surface mounted voltage divider that connects directly to the ring electrodes allowing a fast and easy assembly. This highly modular design enables e.g. the realization of variable drift tube lengths or single and dual gate setups. Instead of the commonly used Bradbury Nielsen gates, the IMS is equipped with a 3-grid ion gate allowing the generation of short (<50 µs) ion packets increasing the resolving power of the instrument.

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Hardware name	Ion Mobility Spectrometer
Subject area	Chemistry and Biochemistry
	 Environmental, Planetary and Agricultural Sciences
	 Educational Tools and Open Source Alternatives to Existing Infrastructure
	• General
Hardware type	 Measuring physical properties and in-lab sensors
	 Biological sample handling and preparation
	 Field measurements and sensors
	 Electrical engineering and computer science
	 Mechanical engineering and materials science
Open Source License	CERN OHL v.1.2 (<u>https://www.ohwr.org/licenses/cern-ohl/license_versions/v1.2</u>)
Cost of Hardware	~\$210 USD for the PCB-IMS and high speed, high gain amplifier
Source File Repository	OSF Link: https://osf.io/p6d4x/Github: https://github.com/bhclowers/OS-IMS

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Warning: Exercise extreme caution when operating and working around the PCB IMS system. Be vigilant regarding the voltage potentials used and the current necessary to drive the unit. Establish appropriate engineering controls to shield the system.

To operate the described PCB IMS it needs to be connected to a high voltage power supply. During operation, conductors at dangerous voltages may be exposed. Extreme care should be taken to protect against shock. Stand on an insulating pad and use only one hand when checking components. Always work with another person in case an emergency occurs. Any work on an operational system should only be executed after the high voltage connectors have been disconnected and the power deenergized.

1. Hardware in context

Ion mobility spectrometry is a gas-phase separation technique that finds utility across analytical domains [1–4]. Most notably, this technique supports many of the field-based detection platforms used to screen passengers, baggage, and goods for explosives and narcotics [5]. Select IMS instruments also find extensive use as point detectors for chemical warfare agents [6]. The wide use of IMS in the field is largely predicated on its relative speed, chemical selectivity, and capacity to operate without expensive vacuum pumps. The sensing principle of IMS is based on a separation of ions by their ion-specific velocity in a drift gas under the influence of an electric field. Compared to other laboratory approaches that probe gas-phase ions, such as mass spectrometry [7], ion mobility systems currently have yet to realize the same levels of resolution. Nevertheless, they serve a critical role as a screening tool. It is important to recognize that the primary role of devices such as IMS is to minimize false negatives where such outcomes are untenable. From a fundamental science perspective, IMS devices also serve as key tools for probing ion-neutral interactions, gas-phase chemistry, and thermodynamic properties of clusters not accessible using other approaches [7–10].

Despite their wide deployment and importance to fundamental science, there are few literature reports detailing the construction and operation of a high-performance, drift-tube ion mobility system. For reference, there are a range of analytical techniques that exploit the property of gas-phase ion mobility to separation ions but the drift tube system arguably provides the largest degree of flexibility, resolution, and accuracy. Conceptually, drift-tube IMS hardware is simple but construction of such devices that produce consistent results has proven challenging and often relied upon a select set of skills, access to resources, and tribal knowledge. In its simplest form, drift tube IMS systems are comprised of an ionization source, reaction/desolvation region, ion gate, drift cell, and detector. Supporting components also include a stable high voltage power supply, ion gating electronics, and a high speed, high-gain current to voltage converter. In the present embodiment of the drift tube IMS, we detail an easily manufactured, open-source drift tube design that incorporates a robust 3-grid shutter design that greatly eases assembly and still enhances performance compared to the traditionally used Bradbury Nielsson Ion gate [11]. In order to maximize the analytical performance, the design process for the size of electrodes, spacers and detector followed the general guidelines given by Bohnhorst et al. [12]. As demonstrated in the latter sections of this report, the IMS system used in this report is capable of attaining resolving powers above 90 for a 10 cm drift cell which exceeds the performance of most commercial systems with a similar footprint. Additional IMS elements included in this design are the drift gas inlet (used to control the local gas-phase environment), detector assembly, and a high-speed, high-gain current to voltage converter. Though a control system is left to the user (a traditional oscilloscope will often suffice), we make recommendations and provide guidance on such tools. It should also be noted that another key element of the drift-tube IMS system not covered in this communication is the ion gate pulser. However, in a separate report [13], we detail the operation and performance of an open-source unit capable of supplying that information.

2. Modular drift tube description and assembly

In this section the assembly of the PCB desolvation and drift region as shown in Fig. 1 is described. In a first step, the electrode alignment board (Fig. 2) is equipped with resistors, specifically surface mount 1206 components. For the presented IMS, $1 M\Omega \pm 1\%$ resistors were used, but more important than the value of the resistor is to consider sufficient voltage ratings. A 10.4 cm drift tube (or desolvation region respectively) consists of 29 electrodes (Fig. 3) and 56 spacers (Fig. 4).

The distance between two electrodes and the inner diameter of the ring electrodes and spacers were chosen according to Bohnhorst et al. in order to realize a homogeneous electric field inside the drift tube enabling to utilize ions within 90% of the inner electrode radius [12]. These design consideration allow the size of the detector to be maximized without broadening of the ion peaks due to field inhomogeneities in close proximity to the electrodes. Therefore, this design leads to an optimum balance between sensitivity and resolving power.

The electrodes and spacers are stacked on rods (we used poly ether ether ketone (PEEK) rods with a 6 mm diameter and threaded ends though any appropriate, non-conducting material would suffice), beginning with an electrode followed by two spacers as shown in Fig. 5. This alternating pattern of 2 spacers to 1 electrode is repeated to achieve the desired drift cell length. Finally, the electrode alignment board is set on top of the stack and the electrode contacts are soldered to the connectors on the alignment board. To achieve higher stability of the setup it is advantageous to connect a second electrode alignment board without resistors to the bottom of the stack. To prevent misalignment of the electrodes and spacers, soldering of the electrode alignment board should only be conducted when the spacers and electrodes are aligned on the

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