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# Computer-controlled, variable-frequency power supply for driving multipole ion guides

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A high voltage, variable-frequency driver circuit for powering resonant multipole ion guides is presented. Two key features of this design are (1) the use of integrated circuits in the driver stage and (2) the use a stepper motor for tuning a large variable capacitor in the resonant stage. In the present configuration the available frequency range spans a factor of 2. The actual values of the minimum and maximum frequencies depend on the chosen inductor and the capacitance of the ion guide. Feedback allows for stabilized, computer-adjustable rf amplitudes over the range of 5–500 V. The rf power supply was characterized over the range of 350–750 kHz and evaluated by driving a quadrupole ion guide in an electrospray time-of-flight mass spectrometer. © *2008 American Institute of Physics.* [DOI: 10.1063/1.2884148]

## INTRODUCTION

The rf-only multipole is the key technology for efficiently transporting ions generated under atmospheric pressure conditions into the high vacuum region of a mass spectrometer. A detailed review of the physics of multipoles and their use as narrow band pass mass filters is available elsewhere.[1,2] Multipole devices consist of two sets of polished, isolated rod pairs set in a parallel geometry within an insulating spacer. rf waveforms, which are 180° out of phase with respect to adjacent rods, are applied to each rod set. In most configurations, a single dc bias potential can also be applied to the rod pairs so that a convenient zero potential can be defined elsewhere within the instrument. Within the multipole, ions are radially focused as they pass along the axis of the device. Transport through the multipole depends on an ion's initial velocity, space charge effects, and the effect of any externally applied field. While moving along the axis of the multipole, ions undergo inelastic collisions with the surrounding buffer gas. The net result is a collimated ion beam at the exit of the device which displays a reduced average kinetic energy and narrowed energy distribution compared to the initial conditions of the ions as they are introduced into the device.[3]

When operated in rf-only mode, multipoles serve as physical high pass filters. For a quadrupole, the low mass cutoff can be approximated from the equations of motion through the device as

$$\frac{m}{z}(\text{minimum}) = \frac{4V}{0.909\omega^2 r_0^2}, \tag{1}$$

where $r_0$ is the inscribed radius of the quadrupole, $V$ is the amplitude of the ac waveform of angular frequency $\omega$, and 0.909 is the $q_u$-intercept value from the Mathieu equations that describe ion motion stability in quadrupoles.[1] The apparent high mass transmission limit of these devices depends on instrumental design and operation parameters, including geometries, pressures, aperture dimensions, voltages applied to electrostatic components, and detection schemes.

For those interested in custom instrument development with atmospheric pressure ion sources or commercial equipment modification, the ion guide and its power supply remain something of a black box. While multipole assemblies can be fabricated in machine shops to satisfy the vacuum and ion optics requirements, appropriate equipment for generating and delivering voltage to these devices is more difficult and expensive to acquire. However, the requirements for the rf power supplies driving rf-only devices are less severe than for multipoles used as narrow band pass mass filters. This is because they are used as high pass filters with a wide mass window relative to the sample of interest. Thus, small changes in the cutoff mass from amplitude and frequency instabilities have limited effects on the final mass spectrum. For example, frequencies ranging from 0.3 to 2 MHz and amplitudes of less than 1 kV are common in devices used in the analysis of biomolecules.[4] The tolerance in frequency and amplitude stabilities is on the order of a few percent. Power supplies used to operate a multipole as a mass filter exceed these specifications and are priced accordingly.

There are three main rf power supply design approaches for driving multipole systems. In the simplest and most expensive design, a high voltage amplifier driven by a function generator can be connected directly to the multipole rods. With this method, the output waveforms from the amplifier match the waveforms on the multipole rods. The multipole represents a purely capacitive load of between 20 and 500 pF depending on its construction. Thus, the multipole ion guide is not an ideal 50 Ω load at typical operational frequencies and this implementation may require an impedance matching network to maximize power transmission efficiency and limit the impact of reflected power on the amplifier. The power requirement for this configuration is large and proportional to the frequency used to drive the ion guide, on the order of >100 W for systems operated at 1 MHz.[5] Due to the large

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power consumption, this design is more useful for applications that require arbitrary waveform generation and not practical for ion guide applications.

The other two designs are based on inductively coupled resonant circuits. An inductively coupled resonant circuit can store energy from a driver system and produce the large amplitude oscillations needed for the ion guide. In the ideal case of efficient energy transfer from the driver to the resonant circuit, the use of a resonant circuit reduces the power demand by a factor of $4Q/\pi$, where $Q$ is the quality factor of the resonant circuit,[5]

$$Q = \frac{f}{\Delta f}. \tag{2}$$

$Q$ values of several hundreds are possible with air core inductors. For looser coupling between the driver and the harmonic system, more power will be required from the driver stage to achieve the same amplitude oscillation. However, a resonant circuit is only able to operate efficiently within a narrow frequency range defined by the $Q$ of the circuit. The resonant frequency for an $LC$ resonant circuit is

$$f = \frac{1}{2\pi\sqrt{LC}}, \tag{3}$$

where the total capacitance $C$ in the system is the sum of the capacitance of the guide, all connection wires, and any added capacitor. Because the harmonic circuit is isolated from the driver stage, the center voltage of the oscillation can be set by an external dc power supply.

The two common implementations of a resonant circuit are a high voltage oscillator and a driven harmonic circuit. High voltage oscillators are usually an $LC$ resonant circuit connected through a transformer to an amplifier with positive feedback. Examples of high voltage oscillators using both vacuum tubes[6] and discrete power transistors[4] as amplifiers can be found in the literature. In these systems, the frequency of oscillation is fixed by the values of the added inductive and capacitive components. Recently, the transistor based design has been improved to take advantage of frequency stabilization techniques.[5,7] One disadvantage to this implementation is that it requires a high voltage power supply and, if implemented on a printed circuit board (PCB), special attention is required due to the high voltages.[8]

The driven harmonic circuit technique is also common.[9] In this method, a low voltage sine wave generator is connected to a power amplifier, which is then used to drive a transformer where the secondary stage is an $LC$ resonant circuit that includes the capacitance of the ion guide. This is similar to a radio, where the transformer is the antenna for an $LC$ circuit that only resonates and amplifies a particular frequency determined by the product of the inductance and the capacitance. The sine wave generator is the radio station that has to send the signal at the frequency set for the $LC$ component. The circuit can be tuned by varying the inductance or the capacitance of the $LC$ resonant circuit or the input frequency from the sine wave generator. An oscilloscope or other rf power measuring device is usually used to tune and to monitor the amplitude of the oscillations on the $LC$ resonant circuit. The main advantage to this design is that only low-voltage components are necessary because the resonant signal from the driver is transferred through the transformer into the $LC$ component, where the power is stored and amplified as defined by the $Q$ of the $LC$ resonator. The greatest drawback to this approach is the cost of the individual components dedicated to signal generation and measurement.

In addition, commercial rf power supplies and published designs that use only fixed components generally operate at a single frequency, but the ability to operate at a wide range of frequencies and amplitudes is of interest for analyzing samples of widely different mass ranges and for the development of custom instruments. Thus, there is a need for a simple and low cost rf power supply for operating ion guides with variable frequencies and amplitudes. In this work, we present a driven resonant circuit designed using commercially available integrated circuits. The circuit is a power function generator that drives a variable resonant circuit. In addition, the design incorporates both negative feedback to maintain stable rf amplitude over the course of operation and power measurement readout enabling software-based frequency tuning. The design is simplified by the use of low voltage (±15 V) components. One key feature of this resonant circuit is the use of an air-variable capacitor that is coupled to a computer-controlled stepper motor to allow software tuning of the $LC$ component and allow oscillation over a factor of 2 in the frequency range. In our implementation of this design, the frequency can be varied between 375 and 750 kHz and the rf amplitude between 5 and 500 V. We evaluate the performance of this design by driving an ion guide in an electrospray ionization time-of-flight mass spectrometer (TOFMS).

## CIRCUIT DESIGN

This circuit is a driven harmonic system composed of a function generator, a low voltage variable gain amplifier, a power amplifier, an output power detector, a power controller, and a transformer/$LC$ resonant circuit. A functional diagram is shown in Fig. 1. dc voltage inputs control both the frequency, and through feedback, the amplitude of the waveform applied to the $LC$ resonant circuit. The output from a sine wave generator is amplified by a regulated low voltage variable gain amplifier and then by a fixed gain power amplifier, which drives the primary stage of a transformer. The energy from the primary stage is inductively transferred to the secondary stage of the $LC$ resonant circuit where the energy is stored, and a high voltage oscillation develops. The $LC$ resonant circuit can be tuned to the frequency of the sine wave generator by rotating the shaft of a variable capacitor. The output waveform is sampled through a capacitive divider, which forms a negative feedback loop with the variable gain amplifier to stabilize the output amplitude.

Figure 2 presents a detailed circuit diagram for the driver and control systems. The role of the voltage controlled function generator is performed by the MAX038 (Maxim Integrated Products, Sunnyvale, CA). The MAX038 is a low cost high frequency waveform generator that functions as a variable relaxation oscillator that creates triangular waveforms of up to 20 MHz by charging and discharging the capacitor

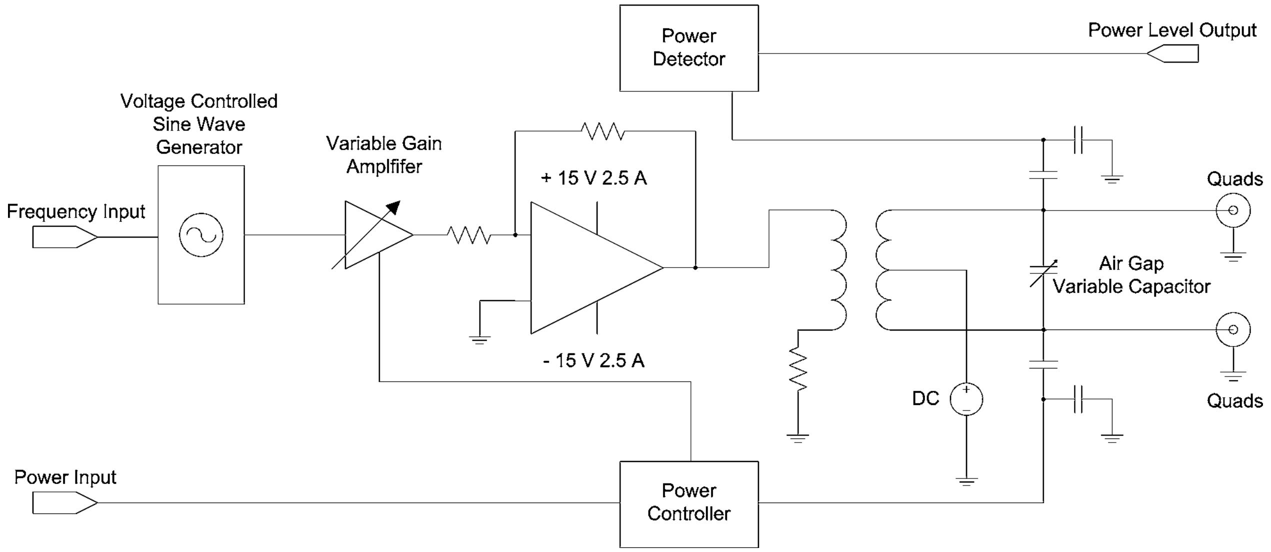

FIG. 1. Simplified schematic of the rf circuit showing all of the functional elements.

connected to pin 5 (COSC). The output frequency is controlled by an input current applied to pin 10 (IIN). Internal circuits shape the triangular waves to produce 2 V peak-to-peak sine waves. In the current configuration, frequency accuracy is approximately 10 kHz, which is sufficient for the rf-only ion guide application. Higher frequency accuracy can be obtained through the use of a crystal reference and a phase locked loop.

Following the signal path, the sine wave output of the MAX038 is then sent through a 1.9 MHz low pass filter (PLP-1.9, Minicircuits, Brooklyn, NY) to remove unwanted high frequency components. The signal is then sent through a 20:1 resistive divider to attenuate it for the dynamic range considerations of subsequent stages. After passing through a buffer stage (OP27, Analog Devices, Norwood, MA) the signal, now a 50 mV sine waveform, is sent to a variable gain amplifier (AD603, Analog Devices, Norwood, MA). The AD603 is a linear-in-decibel amplifier whose gain is con-

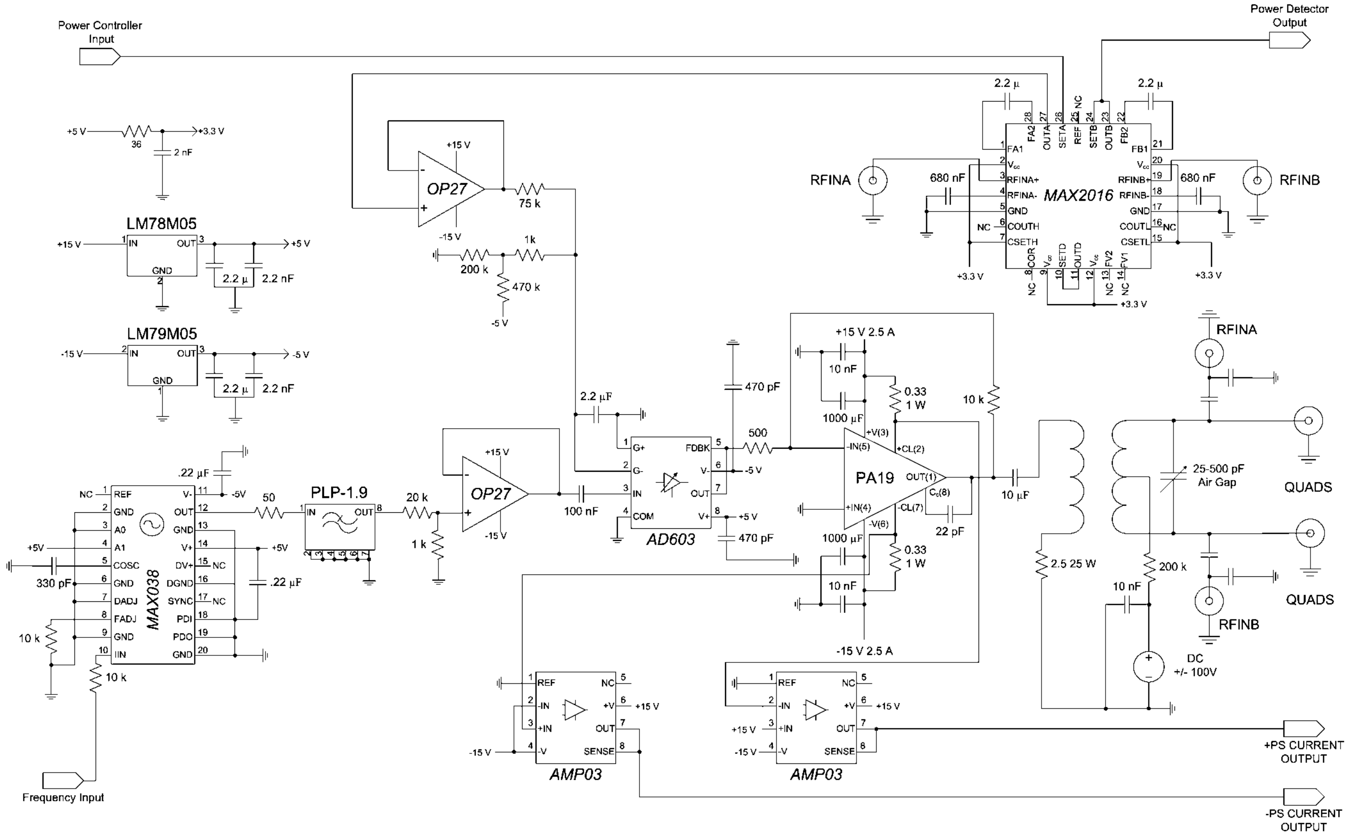

FIG. 2. Detailed schematic of the rf circuit showing the pinouts and connections of the major components.

trolled by a dc voltage input. The amplifier is designed to operate over a −11 to +31 dB range with a gain control of −0.5 to 0.5 V input applied to pin 2 (G−).

In the gain control system, this 40 dB range corresponds to roughly 5–500 V in rf amplitude (10–1000 V peak to peak). The output from the AD603 is then sent to a gain of 20 power amplifier (PA19, Apex Microtechnology, Tucson, AZ).

The PA19 is a high current power amplifier capable of 4 A peak output with ±15 V operation. To protect the amplifier from thermal effects, it was set in a heat sink (HS14, Apex Microtechnology) with a thermal rating of 2 °C/W. The power amplifier drives the primary stage of an air coil transformer which is a small air core inductor with only three turns. This primary stage is wound over and magnetically coupled to a fixed inductor (secondary stage) that forms a resonant *LC* circuit with parallel capacitors composed of the quadrupole rods and coaxial cable connectors (∼100 pF) and a variable capacitor (25–500 pF) (No. 73-1-45-45, Oren Elliott, Edgerton, OH) that can be tuned using a stepper motor. The ratio of minimum to maximum capacitance, resulting from the sum of static and variable capacitors, determines the frequency range over which the supply can be tuned. To achieve the largest possible tunable frequency range, it is most practical to make the minimum capacitance as small as possible because the harmonic frequency of the *LC* resonant circuit exhibits a square root dependence on capacitance. Typically, this involves minimizing the use of coaxial cables and placing the power supply near the ion guide.

The voltage drop across two 0.33 Ω, 1 W resistors and to/from pins 2 and 7 on the PA19 is measured with a pair of differential amplifiers (AMP03, Analog Devices). This voltage drop is proportional to the input current of the amplifier. This current measurement step ensures that the amplifier is being used within the regulated limits of the dc power supply and provides additional information for tuning the circuit and monitoring performance. The 2.5 Ω, 25 W resistor that grounds the primary coil serves to dissipate power from the PA19 and provides a minimum output resistance for the amplifier to drive when the circuit is out of tune.

The voltage on the variable capacitor is sampled with a pair of 1000:1 capacitive dividers and fed into the two inputs of a dual rf detector/controller, MAX2016 (Maxim Integrated Products, Sunnyvale, CA), with 80 dB of dynamic range. One input, RFINB, is used for direct monitoring of the logarithm of the power level on the quadrupole rods. The other input, RFINA, is used as a part of a feedback loop to operate the device in constant power mode. MAX2016 measures the power level of the signal from RFINA using its internal logarithmic detector and compares the power to a set point determined by the dc voltage applied to SETA. The relationship between the measured rf power level and the amplitude of oscillation on the *LC* resonant circuit can be determined experimentally. The MAX2016 increases or decreases the voltage on OUTA to match the power level measurement of the input waveform (RFINA) to the set point voltage (SETA). The OUTA voltage is buffered and summed with a constant voltage at the negative gain control input (G−) of the variable gain amplifier, AD603. This overcomes the restriction imposed by the input/output mismatch of the bipolar AD603, ±0.5 V input, to the single supply MAX2016, 0.5–1.8 V output. By modulating the set point voltage (SETA), it is possible to use the combination of the MAX2016 and the AD630 as a mixer to provide a lower frequency modulation envelope to the output rf waveform. Because the MAX2016 only comes in the QFN surface mount package, it was first soldered to an adapter board (PA-MLF28A-P-S-01, Ironwood Electronics, St. Paul, MN) and then mounted to the main circuit board.

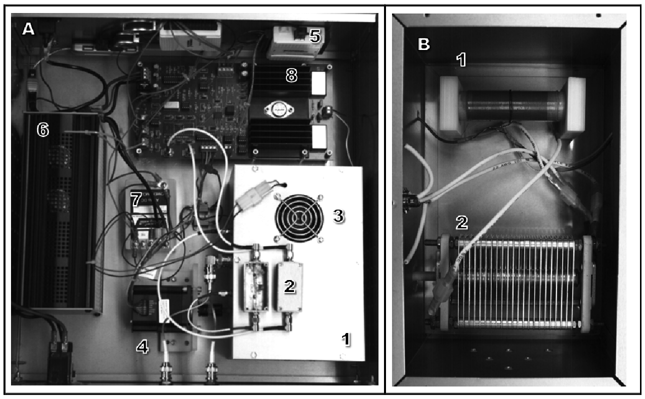

FIG. 3. Photograph of the assembled device. Panel (A) shows the overall system: (A1) Housing for the *LC* component. (A2) Housing for the power detector and controller voltage dividers. (A3) Fan intake. (A4) Stepper motor. (A5) NI 6008 USB interface. (A6) ±15 W, 2.5 A power supply for the PCB. (A7) 24 V power supply for stepper motor and fan. (A8) PCB with driver and feedback electronics. Panel (B) shows the *LC* component enclosed in its own box: (B1) Inductor mounted on a Teflon support. (B2) Variable capacitor. Both of the high voltage elements are mounted on an acrylic plate using Teflon screws. The plates of the variable capacitor are connected to BNC feedthroughs.

Figure 3(a) shows a photograph of the power supply. The low-voltage components of the circuit, with the exception of the capacitive divider and power resistor, are integrated onto a single PCB. A dual tracking ±15 V linear power supply TD15-250 (Acopian, Easton, PA) was used to power the board. The stepper motor and a fan to cool the inductor are powered by a 24 V power supply (24WB125, Acopian, Easton, PA). With the exception of widening the traces for the high current inputs and outputs of the PA19, no special considerations were made in the PCB design. Greater attention to circuit layout might improve the performance of this device by reducing parasitic phenomena. However, we found that our first attempt at designing a PCB provided satisfactory results and did not optimize our design. Two voltage regulators (LM7XM05, National Semiconductor, Santa Clara, CA) provide ±5 V to the components on the board that are designed for lower voltage operation. The entire circuit was installed into a 3U 19 in. rack mountable, alodine-coated aluminum box.

Because the inductor is center tapped, a dc offset can be applied to the ion guide. In principle, any voltage source can be used for this application. In this work, voltage controlled dc/dc convertors (BYH12-100S2 and BYH12-200S1, Bellnix, Saitama, Japan) were used to provide the dc bias voltage. If the center voltage of each end of the coil is con-

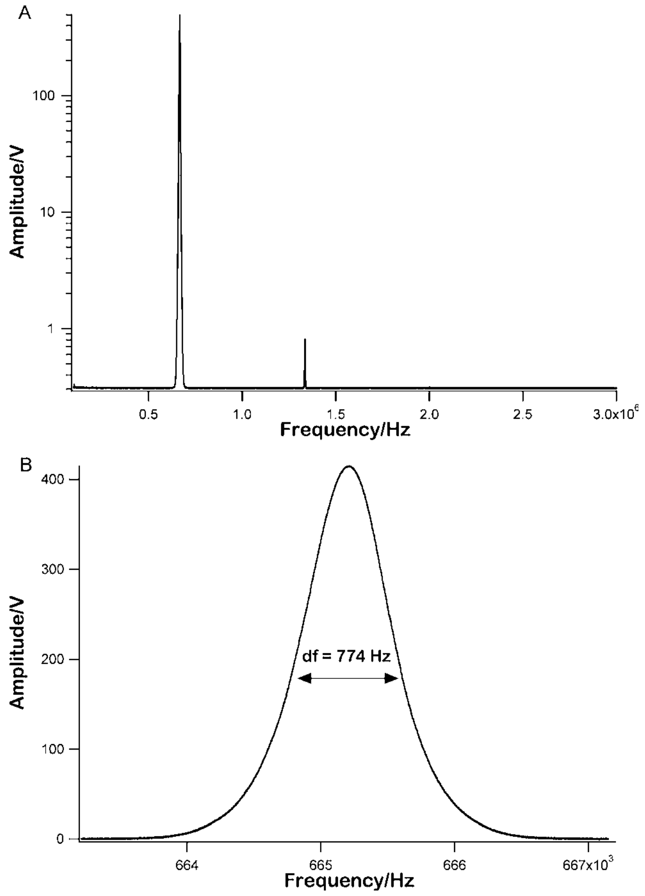

FIG. 4. Performance information on the rf system operating at 665 kHz. (A) Broadband power spectrum from the device output. Only the first harmonic at 1.33 MHz can be seen. (B) Power spectrum showing the width of the output peak at 665 kHz. From this measurement, the $Q$ of the circuit can be determined to be 859.

trolled independently with the use of a second dc/dc converter, then the power supply can be used to drive a multipole for use as a mass filter, where two dc voltages of opposite polarity are applied to the rod sets. To use this circuit as a building block for a precision mass filter would require greater attention to circuit details, especially frequency control and amplitude stability. For this application, a more sophisticated sine wave source may be required that is more stable over time and in response to temperature changes during normal operation.

The power supply is interfaced to a computer through a USB cable using two USB-6008 data acquisition and control modules (National Instruments, Austin, TX). The USB-6008 provides both analog inputs and outputs for controlling the driver stage. The control programming has been written in LABVIEW (National Instruments, Austin, TX).

## rf COIL

Figure 3(b) shows the inside of the housing for the *LC* resonant circuit. The 300 $\mu$H coil used in this work was custom manufactured as a single layer of Litz wire (a type of braided copper wire designed for high frequency applications) by Bournes/J.W. Miller Magnetics (Riverside, CA). The form was placed in a Teflon holder. The coil and variable capacitor were placed within their own alodine-coated aluminum box to limit the effect of radiated rf signal. Because the coil dissipates substantial power during operation at high voltage, a 0.13 A fan was placed over the coil to cool it. The plates of the capacitor are connected to BNC feedthroughs on the outside of the coil box for signal transmission to the ion guide and to SMA feedthroughs for signal transmission to the pair of dividers that lead to the driver board.

The use of a Litz wire inductor is unnecessary for the proper functioning of this circuit. However, a Litz wire coil was used because it was available at the desired inductance and prepared on the correct form size. We have obtained similar results for higher frequency operation by using inductors made by hand winding a single layer of 28 gauge magnet wire against a form made from polycarbonate tubing. The magnet wire was held in place on the form by using fast drying adhesive (LOCTITE 431, Henkel Corporation, Rocky Hill, CT). The inductance of single layer coils can be approximated using an equation from a handbook.[10]

## VARIABLE CAPACITOR AND FREQUENCY TUNING

The resonant circuit can be turned by rotating the shaft of a variable capacitor using a stepper motor (23MD, Anaheim Automation, Anaheim, CA). TTL pulses to drive the rotation of the stepper motor are provided from the digital outputs of one of the USB-6008 modules. The shaft of the capacitor, which is held at the voltage of the oscillation, is mated to the shaft of the stepper motor using a polymer coupler insert. The resonant frequency of the *LC* circuit changes with the angular position of the capacitor shaft and the output is maximized when the frequency matches the fixed output frequency from the MAX038 function generator. In our current implementation with a 300 $\mu$H coil, a tunable range of 375–750 kHz can be achieved. Because of the symmetry of the capacitor, it is possible to tune the *LC* circuit for intermediate frequencies at two positions of equal capacitance. At the ends of the frequency range, which correspond to the minimum and maximum capacitances possible, only a single position on the capacitor satisfies the criterion for resonance.

During normal operation, tuning is achieved in a two step process. To rapidly tune the power supply, the rf amplitude is set to a minimum and the motor is stepped in full 1.8° steps until a threshold voltage is met. Above the threshold voltage, the motor moves forward in $\frac{1}{8}$ steps (0.225°), recording the voltage versus step number in memory. After the output voltage begins to decrease, the motor steps backward to the position of the recorded maximum. Once tuned, the system can be operated for several days without retuning. However, once the power supply is deenergized, the stepper motor loses its holding torque and the mated shafts can rotate out of the tuned position.

## PERFORMANCE

The output characteristics of the power supply were evaluated using a spectrum analyzer (HP 8590L, Agilent Technologies, Santa Clara, CA) and detailed in Fig. 4(a). In this test, the power supply was disconnected from the ion

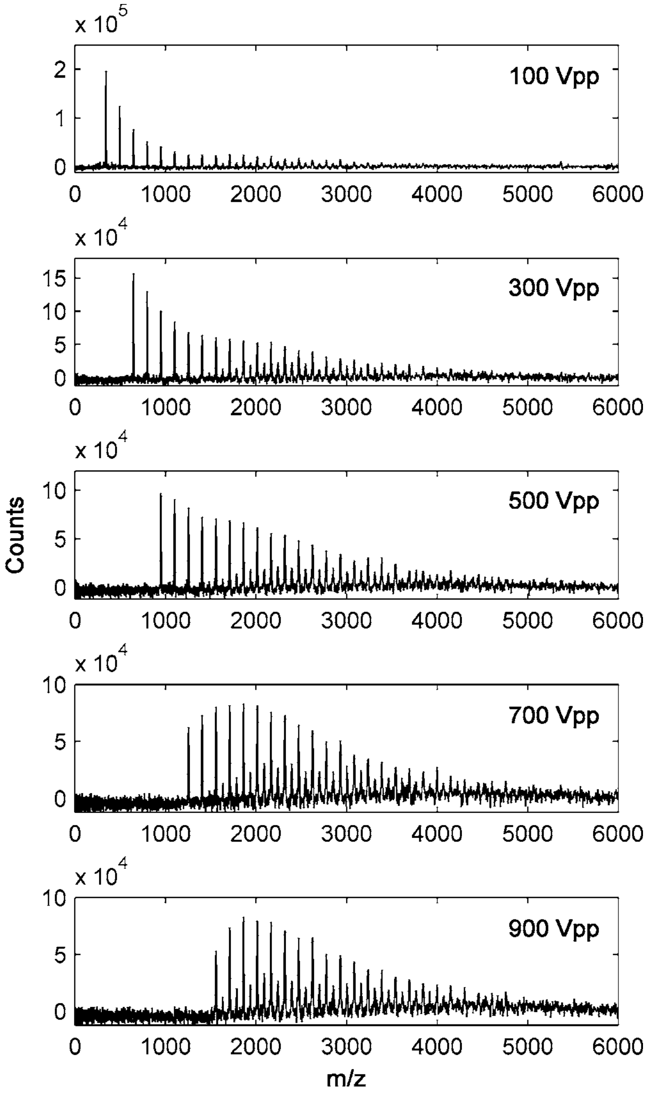

FIG. 5. Electrospray mass spectrum of potassium trifluoroacetate produced from a 50/50 $v/v$ mixture of acetonitrile and water at a flow rate of 2 $\mu$l/min. A potential of 3.5 kV was applied to the 50 $\mu$m inner diameter stainless steel electrospray emitter.

guide and one of the high voltage outputs was connected to a high voltage probe (N2271A, Agilent Technologies) and fed into the 8590L. The measured voltage was corrected by a factor measured against the 1 M$\Omega$ vs 50 $\Omega$ input of an oscilloscope (LT342, LeCroy, Chestnut Ridge, NY). From the figure, it is shown that the output waveform is clean and does not contain spurious frequencies, and the impact of higher harmonics is limited. Because the *LC* circuit is operating as a filter, the output spectrum is cleaner than for rf power supplies that function as high voltage oscillators. However, for the ion guide application, this is likely irrelevant. The $Q$ factor of the *LC* circuit could be measured from the spectrum analyzer and was shown to be approximately 890 at 680 kHz [Fig. 4(b)].

The use of the power supply to drive an ion guide was tested by acquiring mass spectra on a homebuilt linear TOFMS. The instrument was constructed around an atmospheric pressure ion source salvaged from a Mariner TOFMS (PerSeptive Biosystems, Framingham, MA). The principles of operation for this device are described elsewhere.[11–13]

A common calibration compound, potassium trifluoroacetate, was chosen for this experiment because it provides a large number of evenly spaced peaks over a wide mass range.[14] In this experiment, the quadrupole ion guide was operated at 665 kHz and the ion abundances of the beam exiting the ion guide were measured at different rf amplitudes. The results appear as Fig. 5. The peaks that appear are $(F_3CCOO^-K^+)_n(K^+)_z$ clusters. The most prominent peaks are attributed to the $z=1$ clusters. At the lowest rf amplitude, the peak series begins with the $n=2$ peak. At higher rf amplitudes, lighter $z=1$ clusters are not transmitted because of high pass filtering effect. Clusters with $z=2$ can be seen and peaks detected up to 5000 Da. A more detailed analysis of the data shows $z>2$ clusters near the base line of the data. One particular advantage associated with the high pass filter phenomenon for TOFMS is the elimination of chemical noise from atmospheric ion sources that may appear in the region corresponding to species with low mass-to-charge ratios.[15] Here the movement of the low pass limit can be seen by the disappearance of the lowest cluster peak for every 100 V increase in rf amplitude.

In summary, we have developed a tunable frequency and amplitude rf power supply for driving a multipole ion guide using integrated circuits and a stepper-driven variable capacitor. The design and implementation of this device are simplified by the use of integrated circuits in the driver stage. The flexibility of this power supply combined with its low cost should enable future work on custom instrumentation for mass spectrometry.

## ACKNOWLEDGMENTS

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