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A simple and cost-effective high voltage radio frequency driver for multipolar ion guides

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Abstract

Multipolar RF ion traps are widely used in mass spectrometry for guiding ion beams and are fundamental tools to study ion-molecule reactions in the near thermal and sub-thermal regime. A flexible, cheap and reliable RF power source can be obtained by using a home-made matching network to couple the ion guide to a commercial RF power supply.

In this paper we describe the design and the construction of a RF power supply for driving two octopole ion guides at the same time. Details on the design and the practical building of the matching network are discussed.

Performances of the apparatus are demonstrated by measuring transmission curves for Helium, Neon and Argon ions. © 2007 Elsevier B.V. All rights reserved.

Keywords: RF; Octopoles; Ion guides

1. Introduction

Multipolar ion guides operating in the radio frequency (RF) regime are widely used in mass spectrometry for trapping and guiding ions. They trap charged particles in two dimensions, allowing them to travel along the longitudinal axis of the guide. Experiments carried out with slow ions take advantage of ion guides to compensate space charge effects, which represents the actual limit for the production of low energy ion beams. In addition, ion traps are used in scattering and spectroscopy experiments to increase the overall sensitivity [1–7].

Since RF ion guides can operate at relatively high pressures [2], they can also be used to thermalize ions by means of inelastic collisions with a suitable buffer gas [8]. A possible development of this approach envisages the use of chemically active molecules for preparing state-selected ion beams.

An ion guide consists of two sets of electrodes with axial symmetry, powered by sinusoidal voltages opposed in phase. Ions are trapped due to their oscillation in the inhomogeneous time dependent electric field. The amplitude and the frequency of the supplied voltage depend on both the geometry of the trap and the mass-to-charge ratio of the trapped ions. The theory of operation is well established and has been reviewed in several papers [3,6,9,10]. Neglecting the high frequency component of the ion trajectories, the trapping effect of the RF electric field can be described, as a function of the distance from the center of the trap (r), by a time independent, effective potential V_{eff}

$$V_{\rm eff} = \frac{n^2}{4} \frac{V_0^2}{r_0^2 \Omega^2} \frac{q^2}{m} r^{2n-2}$$
(1)

where 2n is the number of poles of the trapping device, r_0 is the inner radius of the ion trap, V_0 is the peak amplitude, Ω ($\Omega = 2\pi f$) is the angular frequency of the RF voltage, *m* and *q* are the mass and the charge of the trapped particle.

The range of validity of this approximation is defined by the adiabaticity parameter η that has to be lower than 0.3

$$\eta = 2n(n-1)\frac{V_0}{r_0^2 \Omega^2} \frac{q}{m} r^{n-2}$$
(2)

The RF power supply of the ion guide can be designed in several ways. For low frequency applications ($f \le 500 \text{ kHz}$) direct drive is a possible solution, but at higher frequencies effects due to the

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capacitive load of the circuit limit the use of such an architecture. The problem can be partially overcome if the guide itself is part of a resonant circuit [2,5,9,11–14]. Then, in principle, the required power is only that necessary to reintegrate the losses of the resonant circuit, but, in practice, the amount of electric power transferred to the guide depends critically on the tuning of the circuit. The resonant circuit can be designed in two ways. In the first way, an external power source, made by a RF generator and an amplifier, is coupled to the guide electrodes by a matching network which tunes the impedance of the trap with the output impedance of the amplifier, maintaining at the same time resonance conditions [5]. Alternatively, the capacitive load of the ion guide is the actual capacitance of a resonant circuit [9,11–14] and the driver does not require any matching network. In this case the electric field does not oscillate at an a priori fixed frequency, since the system undergoes a sort of autotuning. This solution has been proposed some years ago by using a tube oscillator [11,12,14] while, more recently, the scheme has been realized by a resonant switching design [9,13]. The performances are good, but this system requires some dedicated electronics which is not readily available, in particular when high output power is required. On the contrary, the scheme that uses the matching network is simpler and it can be realized to a great extent by assembling commercial products. In addition, a well designed matching network behaves as an efficient band-pass filter, thus providing a neat sinusoidal voltage on the electrodes. The overall design of the RF power supply is therefore almost independent on the level of distortion of the power stage and this results in a cost-effective project, since one can use a common radio transmitter for the power source. In this case the overall problem reduces to the realization of the matching circuit.

In this paper we describe the design of a Dual High Voltage Matching Network (DHVMN) that couples a commercial broadband RF amplifier to an ion guide system composed by two octopole guides working at 13.56 MHz, the standard laboratory RF frequency which avoids interferences with radio communications. The system is part of a tandem spectrometer used for studying ion-molecule reactions [2,14].

The combined use of multiple ion guides in the same experimental set-up is useful for a variety of mass spectrometric applications. While the most common application consists in guiding slow ion beams, RF guides can be also combined to perform (a) cooling stages for quenching excited states by collisions with a suitable buffer gas [8], (b) collision cells [2,4,5], (c) kinetic energy analyzers based either on Time Of Flight (TOF) or retarding field sections [5,14]. In the former applications, keeping the same phase on all the ion guides may be an advantage. Indeed, every phase mismatch between the two ion guides affects the reliability of the experimental data since the ions can be accelerated in the transition region between the two ion guides.

2. Design

2.1. Specifications

The coupling network between the ion guide and the RF power generator has to:

- match the impedance of the guide load to that of the RF generator;
- realize a resonant high Q circuit to power the guide electrodes;
- provide two sinusoidal waveform with the same frequency and in phase opposition;
- provide a DC bias voltage for the guide with respect to ground.

The DHVMN hereafter proposed fulfills these requirements and has the following advantages:

- its construction is simple and cheap;
- it can be coupled even with cheap RF amplifiers presenting high distortion levels;
- it does not require a sophisticated transformer as the performances of the circuit do not depend critically on the coupling between the transformer inductances;
- it can be easily adapted to every reactive load with low losses. This makes it an ideal solution to power different types of ion traps.
- the output voltage can be controlled by varying the input power.

2.2. Circuit design and simulations

A schematic view of the DHVMN is reported in Fig. 1. The two octopoles appear as capacitors (Oct₁ and Oct₂). A DC bias voltage can be set by Vdc₁ and Vdc₂ power supplies. The inductance marked "L choke" coupled with the capacitors "Cg₁" and "Cg₂" prevent the RF voltage from reaching the DC bias power supplies. " C_{block} " capacitors allow to set an independent DC bias on the two ion guides.

In operating conditions the matching network have to be in resonance at the chosen frequency with a total input impedance of 50 Ω . In principle these conditions can be obtained by regulating either the capacity or the inductance. However, since the impedance of the system octopoles + cables is mainly capacitive, it has to be compensated by inserting an additional inductance (L_p). Fine tuning is then achieved by means of the C_1 , C_{s_1} and C_{s_2} variable capacitors (see later on).

By defining X_{C_0} the reactance of the system composed by the cables and the octopoles, the total reactance of the load X_{load} can be obtained by resolving the parallel circuit between X_{C_0}



Fig. 1. DHVMN scheme.



Fig. 2. RLC equivalent circuit.

and X_{L_p}

$$\overline{X_{\text{load}}} = \frac{\overline{X_{C_0} X_{L_p}}}{\overline{X_{C_0} + \overline{X}_{L_p}}}$$
(3)

Considering that X_{C_0} is capacitive, to obtain an inductive X_{load} it is necessary to have

$$|\overline{X_{C_0}}| > |\overline{X_{L_p}}|$$

In these conditions, the circuit in Fig. 1 can be reduced to the equivalent circuit shown in Fig. 2, where R_1 and R_2 summarize the losses, *L* is an inductive load with reactance X_{load} and C_s is the series of C_{s_1} and C_{s_2} .

It is worth noting that if one wants the voltage on the octopole rods to be as large as possible, then the potential drop across Lhas to be as large as possible, since this value is proportional to the actual potential difference between the octopoles rods. To achieve these results it is necessary to put

 $|\overline{X_{C_0}}| \approx |\overline{X_{L_p}}|$

this conditions fixes the value of L_p .

The determination of the electrical parameters to fulfill the above specifications requires the solution of the system of the two Kirchhoff equations (for the primary and secondary circuit), which are coupled by the mutual induction of the transformer M

$$\begin{cases} \overline{V_1} = \overline{Z_1} \cdot \overline{I_1} - j\omega M \overline{I_2} \\ 0 = \overline{Z_2} \cdot \overline{I_2} - j\omega M \overline{I_1} \end{cases}$$
(4)

$$\overline{Z_1} = R_1 + j(X_{L_1} - X_{C_1}) = R_1 + jX_1,$$

$$\overline{Z_2} = R_2 + j(X_{L_2} + X_L - X_{C_s}) = R_2 + jX_2$$

Resolving for the electrical parameters of the primary circuit it is possible to calculate the impedance transferred to the primary one Z_{21} . The previous system reduces to

$$V_1 = (Z_1 + Z_{21})I_1$$
$$\overline{Z_{21}} = \frac{\omega^2 M^2}{\overline{Z_2}} = \alpha + j\beta$$

where α and β represent the resistance and the reactance transferred from the secondary circuit to the primary one, respectively.

For α it follows

$$\alpha = \frac{\omega^2 M^2 R_2}{R_2^2 + X_2^2}$$
(5)

From this equation it's clear that the resistance transferred to the primary circuit (α) depends on the mutual induction of the transformer *M*, the resistance R_2 and the reactance X_2 of the secondary circuit.

The constrain on the output resistance R_a of the RF amplifier fixes the value of α , given the measured value of R_1

$$\alpha = R_{\rm a} - R_{\rm l} \tag{6}$$

From Eq. (5) and condition (6) one obtains for X_2

$$X_2 = \pm \sqrt{\frac{\omega^2 M^2 R_2}{\alpha} - R_2^2} \tag{7}$$

Since α is fixed by Eq. (6) and R_2 is estimated from the actual circuit, the previous relation can be used to calculate X_2 given the value of M, the latter one being measured after the construction of the transformer. It is important to point out that the realization of the transformer does not need to satisfy strict specifications for L_1 , L_2 and K (K = coupling coefficient, $M = K\sqrt{L_1L_1}$) since for a wide range of M it is possible to find a value for X_2 that gives perfect tuning. The only condition which has to be fulfilled arises from the limit on the transferred resistance α . Since for a given R_2 value the maximum α is obtained for X_2 =0, one obtains from Eq. (7)

$$M > \frac{1}{\omega} \sqrt{R_2 \cdot \alpha}$$

By fixing X_2 from Eq. (7) it is possible to resolve the overall circuit.

Assuming X_2 capacitive (negative solution), it is possible to derive C_s by the relation

$$X_{C_{\rm s}} = X_L + X_{L_2} - X_2$$

The resonance condition fixes the value of C_1 by the relation

$$X_{C_1} = X_{L_1} + \beta \tag{8}$$

From Eq. (4) it is possible to determine the value of the secondary current I_2

$$\overline{I_2} = j \frac{\omega M}{\overline{Z_2}} \overline{I_1}$$

That in resonance, see Eqs. (8) and (7), becomes

$$|\overline{I_2}| = \sqrt{\frac{\alpha}{R_2}} \cdot |\overline{I_1}| = \sqrt{\frac{\alpha}{R_2}} \cdot \frac{|\overline{V_1}|}{R_a}$$

One request of the design is to minimize the input power. Power losses in the circuit are due to the non-ideal behavior of the circuit components at the working frequency. In our design these effects have been summarized by R_1 and R_2 . Their values have been estimated by measuring with an LCR meter the serie resistances associated with every circuital element at 13.56 MHz. To maximize the efficiency of the circuit it is necessary to minimize R_1 and R_2 and this can be obtained by selecting low-losses components for the realization of the DHVMN. Power losses are particularly significant for the inductor L_p which have to be realized by choosing low-losses materials.



Fig. 3. Simulated circuit. Note that in contrast to the actual circuit shown in Fig. 1, in the simulated circuit only one inductance is connected to Oct1, since the Simulation Software does not permit a double connection with two points at the same potential. However, the above scheme is a good approximation since the "L choke" value does not perturb the tuning of the circuit.

On the bases of this general scheme, the actual design of the DHVMN has been defined and simulated. The requested operating conditions are: frequency of 13.56 MHz, cables length of 1.2 m, input impedance of 50 Ω and peak to peak voltage between the trap electrodes 1 kV. A schematic picture of the circuit is shown in Fig. 3. The electric characteristics of the octopoles can be identified by measuring the capacity CL_e between the two electrode systems (each composed by four rods) and from each electrode system and ground CL_{g1}, CL_{g2}

- Octopole one: $CL_e = 40 \text{ pF}$; $CL_{g1} = CL_{g2} = 70 \text{ pF}$.
- Octopole two: $CL_e = 45 \text{ pF}$; $CL_{g1} = CL_{g2} = 60 \text{ pF}$.

These values can be reduced to an equivalent capacity of 75 pF for both octopoles (CL₁ and CL₂, respectively). The transformer has the following characteristics: $L_1 = 0.4 \,\mu\text{H}$, $L_2 = 1.1 \,\mu\text{H}$, K = 0.6. The values for the resistances R_1 (1 Ω) and R_2 (19 Ω) have been evaluated by an LCR meter and they take into account the non-ideal behavior of all the components at the selected frequency.

With these constraints the circuit has been resolved. We have simulated the performances of the system with the "Circuit-Maker's Berkeley SPICE3f5/X" Spice-based simulator with a realistic set of operating conditions: with 73 V (peak to peak) for V_1 we get a voltage of 1 kV peak to peak with the right phase on the bars of both the octopoles.

The DHVMN has been built almost completely by using standard electronic components (C_1 , C_{s_1} and C_{s_2} are air variable capacitors). The only non-commercial one is the home-made RF transformer. Primary and secondary coils ($L_1 = 4$ windings, $L_2 = 6$ windings) are air coupled and have been constructed with a standard 2 mm² copper wire mounted around a plastic tube ($\emptyset = 30$ mm). A small cooling fan makes more efficient heat dissipation. A picture of the DHVMN is shown in Fig. 4.

The DHVMN is powered by a commercial 200 W broadband (3–30 MHz) amplifier (MICROSET 27-200 T) used for radio communications. In our case the input RF signal is provided by a home built oscillator (0–5 W output power) which guarantees a small power deliver to the input stage of the RF amplifier. Bias voltages on the octopoles are provided by two commercial DC power supplies (Vdc₁ and Vdc₂).

To monitor on-line the tuning level it is useful to introduce a Rosmeter between the amplifier and the DHVMN, while two low capacity oscilloscope probes can be used to check the voltages directly on the ion guide or at the exit of the matching network. It is important to point out that, regardless their characteristics, the two probes can perturb the circuit and tuning conditions may change when they are removed, so it is better to have them symmetrically positioned on the circuit and grounded separately.

RG58 C/U cables have been used for the transmission line delivering the voltage from the DHVNM. Electrical connections under vacuum are made by commercial RF wires inserted inside a ceramic tube for insulation (length about 30 cm); connections between the inside and the outside of the experimental set-up are realized with commercial RF feed through. Octopoles are made by stainless steel rods ($\emptyset = 1 \text{ mm}$) mounted on ceramic insulators, the first one have an inner diameter of 9 mm and a length of 82 mm, the second a diameter of 6 mm and a length of 102 mm.

The tuning of the system is achieved acting on the capacitors C_1 , C_{s_1} and C_{s_2} . By regulating C_{s_1} , C_{s_2} it should be possible to obtain two sinusoidal voltages in phase opposition with a negligible reflected power on the Rosmeter. This last parameter



Fig. 4. Picture of the DHVMN.

can be further adjusted by acting on C_1 . Due to the coupling between the primary and secondary circuit, after each regulation of C_1 it is necessary to re-adjust C_{s_1} , C_{s_2} .

3. Performance

The operation of the power supply has been tested by driving the two octopoles of our Guided Ion Beam (GIB) [2,14] apparatus. The GIB mass spectrometer allows cross section measurements for reactions of ions with neutral molecules. The primary ion beam is produced by electron bombardment and can be collisionally relaxed into the first octopole ion guide. It is subsequently mass-selected by the first quadrupole mass spectrometer. Reactant ions are injected into the second octopole ion guide, which is surrounded by the scattering cell filled with target molecules. The gas pressure in the cell can be regulated, in the range 10^{-7} to 10^{-2} mbar. The ion beam energy can be varied by changing the octopole bias (DC) potential with respect to the ion source, and this permits measurements as a function of the collision energy. Reactant and product ions are analyzed by the second quadrupole mass spectrometer and finally detected.

The trapping efficiency of the second octopole, which is used for measuring ion-molecule reaction rates, has been characterized by using ion beams of different rare gases (He, Ne, Ar). The beam intensity has been measured on the conical lenses used to inject the ions in the octopole (I_{in}) and on the extraction lenses after the ion guide (I_{out}). Since only a fraction of I_{in} reach the ion guide, the ratio I_{out}/I_{in} is proportional to the actual transmission efficiency of the octopole. The dependence of this parameter on the peak-to-peak RF voltage (V_{p-p}) applied on the rods is shown in Fig. 5. In all the cases experimental data show an increase of the trapping efficiency followed by a nearly constant region. For Argon it extends from 200 to 700 V which is the actual limit of our system, while Neon transmission starts flattening earlier at 150 V. In the case of Helium the situation is somewhat different. The initial increase of the ratio I_{out}/I_{in} is faster while the constant region extends only up to 300 V, followed by a decrease of the ion current.



Fig. 5. Transmission curves for Helium, Neon and Argon. Ratios between the ionic current measured on the ion optics before (I_{in}) and after (I_{out}) the octopole are plotted as a function of the peak-to-peak RF voltage (V_{p-p}) applied to the trap electrodes. This ratio is proportional to the actual transmission efficiency of the octopole. Error bars are due to statistics on the experimental data.

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Values for the effective potential and the adiabaticity parameter at the inflection point value of the voltage in Fig. 5 (see text)

Ion	$V_{p-p}(V)$	$V_{\rm eff}~({\rm eV})$	η
Ar ⁺	200	1.5	0.09
Ne ⁺	150	1.66	0.13
He ⁺	90	3	0.4

Experimental results have been analyzed by comparing them with calculations for the effective potential V_{eff} and for the adiabaticity parameter η . Their values for the voltages corresponding to the inflection point in Fig. 5 are shown in Table 1.

In the experimental set-up, the injection of the ions into the octopole is performed by a conical lens that limits the angular divergence of the ion beam at 41°. Experimental data shown in Fig. 5 have been recorded at an ion kinetic energy of 3.5 eV in the laboratory frame of reference. By using the values for the effective potential reported in Table 1, it is straightforward to estimate the divergence of the ion beam by setting the effective potential to be equal to the radial kinetic energy of the ions. For Ar and Ne the calculated angular divergences turn out to be 41° and 43° , respectively, in substantial agreement with the geometric limit of 41°. For He such divergence is different as the calculated divergence is 68°. This result can be rationalized by considering that in this case the value 0.4 for the η parameter is much larger than the recommended value for safe operation $(\eta = 0.3)$ and therefore adiabaticity conditions are not fulfilled. In the case of He⁺ this condition can be satisfied by increasing the frequency of the octopole driver.

4. Conclusions

In this paper we describe the design and construction of a RF power supply system able to drive multiple ion guides. We discuss in details the electronic design and the practical realization of a coupling stage between a commercial broadband RF amplifier and a two octopole ion guide used for studying ion–molecule reactions. Our scheme shows good performances in terms of stability, reliability and collection efficiency, being at the same time simpler and more cost-effective than other solution proposed in literature. These features allow its implementation even in laboratories which lack a specific background in advanced electronics and can contribute to a widespread use of ion guides.

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References

[1] O.V. Boyarkin, S.R. Mercier, A. Kamariotis, T.R. Rizzo, J. Am. Chem. Soc. 128 (9) (2006) 2816.

- [2] G. Guella, D. Ascenzi, P. Franceschi, P. Tosi, Rapid Commun. Mass Spectrom. 19 (14) (2005) 1951.
- [3] D.J. Douglas, A.J. Frank, D. Mao, Mass Spectrom. Rev. 24 (1) (2005) 1.
- [4] P. Armentrout, Threshold Collision-Induced Dissociations for the Determination of Accurate Gas-Phase Binding Energies and Reaction Barriers. Topics in Current Chemistry, vol. 225/2003, Springer Berlin/Heidelberg, 2003, p. 233.
- [5] O. Dutuit, C. Alcaraz, D. Gerlich, P. Guyon, J. Hepburn, C. Metayer-Zeitoun, J. Ozenne, M. Schweizer, T. Weng, Chem. Phys. 209 (1996) 177.
- [6] D. Gerlich, State-Selected and State-to-State Ion-Molecule Reaction Dynamics, Part 1: Experiment, vol. LXXXII of Advances in Chemical Physics, John Wiley and Sons Inc., 1992, p. 1.
- [7] P. Tosi, Chem. Rev. 92 (1992) 1667.

- [8] T.M. Bernhardt, J. Hagen, L.D. Socaciu, R. Mitric, A. Heidenreich, J.L. Roux, D. Popolan, M. Vaida, L. Woste, V. Bonacic-Koutecky, J. Jortner, Chem. Phys. Chem. 6 (2005) 243.
- [9] I. Cermak, Rev. Sci. Instrum. 76 (2005) 063302.
- [10] P. Tosi, G. Fontana, S. Longano, D. Bassi, Int. J. Mass. Spectrom. Ion Proc. 93 (1989) 95.
- [11] R.M. Jones, S.L. Anderson, Rev. Sci. Instrum. 71 (11) (2000) 4335.
- [12] R.M. Jones, D. Gerlich, S.L. Anderson, Rev. Sci. Instrum. 68 (9) (1997) 3357.
- [13] P.B. O'Connor, C.E. Costello, W.E. Earle, J. Am. Soc. Mass. Spectrom. 13 (2002) 1370.
- [14] O. Hadjar, D. Ascenzi, D. Bassi, P. Franceschi, M. Sabido, P. Tosi, Chem. Phys. Lett. 400 (2004) 476.