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Properties of a multipole ion trap studied by evaporative ion losses

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ABSTRACT

We have studied a scheme for analysing the effective trapping potential for ions in a 22-pole ion trap, based on the strong dependence of the lifetime of the ions on the buffer gas temperature. We distinguish two regimes for ion losses, either over one of the two end cap electrodes (axial direction) or over the effective radiofrequency potential (radial direction), and examine these schemes under different trap settings. We have found that evaporation over one of the end caps yields an effective temperature of the ions that is much larger than the buffer gas temperature. This may be a hint for an enhancement of the high-energy tail of the ions' velocity distribution. We also observe and investigate a breakdown of thermalisation for trap temperatures lower than 25 K. Measurements for OH^- and D^- anions have shown that this feature is independent of both the buffer gas to ion mass ratio and the trapping parameters.

1. Introduction

Investigations of ion-molecule reactions require internally and translationally thermalised ions with a well defined temperature. Cold molecular ions are also desired for spectroscopy studies. The widely used techniques for cooling atomic ions are not applicable for molecular ions. Laser cooling is generally not applicable because of the lack of the closed optical cycling transitions. Sympathetic cooling with laser cooled atomic ions has no influence on the internal energy distribution of molecular ions [1,2]. Only collisions with neutral buffer gas cool both internal and external degrees of freedom (see for example [3,4]). High order multipole traps such as the 22-pole trap [5] are very suitable for such ion preparation [6,7]. They have a large field free region and as a result strongly reduced radiofrequency (rf) heating and long ion lifetimes. There exist a number of temperature measurements of molecular ions in a 22-pole trap, most of them based on spectroscopy [3,4,8–13]. These measurements indicate the existence of a discrepancy between ion temperature and buffer gas temperature for both internal and external degrees of freedom. Most of them are based on bound-bound action spectroscopy and can not easily be generalised to arbitrary molecular ions and anions in particular.

In this paper we analyse ion losses of OH^- and D^- from a 22-pole trap in the radial and axial directions and the role of such factors as different ratios between buffer gas mass and ion mass and distortions of the trap potential. We can also extract an effective translational temperature from the loss rate measurements for OH^- and we discuss the observed deviations when comparing with the buffer gas temperature.

2. Experimental procedure

A detailed description of our experimental setup can be found in [14]. Each experiment includes the following basic steps: ion production, selection of certain species, trapping, cooling, extraction and detection of ions.

Ions are produced in a pulsed-gas discharge source and are extracted with a Wiley–McLaren mass spectrometer. Then the preselected ions are stored in a 22-pole trap. A schematic view of the trap that we use in our experiments is shown in Fig. 1. It consists of 22 stainless steel rods (1 mm diameter, inscribed diameter 10 mm) alternatingly connected at the axial end plates to the two outputs of an rf oscillator providing a cylindrically symmetric effective potential in the radial direction. For confinement in the axial direction, we have a set of four ring electrodes. The inner end caps are used to confine the ions in the axial direction and the outer caps are optimised for loading and extraction of the ions. All four end cap electrode potentials have a significant influence on the final potential barrier height. Loading the trap with end cap voltages in the millivolt regime has proven difficult. To trap ions efficiently in this case we apply −10 to −15 V on the inner end caps (measured with respect to the trap DC potential) during the initial thermalisation

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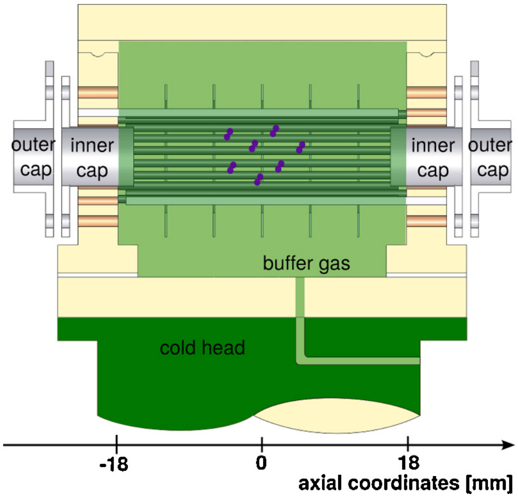

Fig. 1. 22-Pole rf ion trap consisting of 22 rf electrodes for radial confinement (arranged at an inner diameter of 10 mm) and of two pairs of cap electrodes in the two axial directions. The trap is mounted on a cold head and surrounded with the thermal radiation shielding (not shown). The five vertical shaping lenses placed around the rf electrodes are set to the same potential as the DC potential of the trap.

time. Then the voltage is slowly ramped down to the chosen voltage by using an RC filter with a time constant of 0.7 ms.

Once the ions are in the trap they undergo collisions with buffer gas (He, D_2 or H_2) and as a result cool down translationally and internally. The typical buffer gas density in our experiments is on the order of 10^{13} cm^{-3}. Assuming a Langevin-limited collision rate, ions undergo 10^3-10^4 collisions per second and their thermalisation time is of the order of 10 ms.

After a storage time (typical values are in the range of less than 1 to beyond 100 s), the ions are extracted from the trap and are detected. We repeat this procedure for different values of the storage times and fixed parameters (temperature, buffer gas density, the trap potentials) and obtain the dependence of the ion signal on the trapping time. An exponential fit to this data yields the loss rate.

To explore evaporative losses of the ions from the trap, we measure the loss rate for different trap temperatures. The buffer gas temperature is fixed by collisions with the trap walls. The trap itself is mounted on a closed cycle cryostat (Leybold Coolpak 4000) and can be cooled down to 10 K. It is surrounded by thermal radiation shielding to minimise heating by blackbody radiation. Ohmic heaters allow us to vary the trap temperature between 10 K and room temperature. To minimise the influence of impurities vaporised during heating, all measurements have been performed within the cooldown phase of the trap.

For comparison with the experiment we simulate the potential landscape of the ion trap with the SIMION software [15] based on the finite difference method. As a result, we obtain a number of potential arrays, each of which contains information about one electrode. Based on these arrays, the electric field can be obtained at any location inside the trap for any combination of electrode voltages. The effective potential corresponding to the rf voltage and the electrostatic field of the end caps have been obtained separately and later superimposed. The effective potential has been obtained from [7]:

$$V_{eff}(\vec{r}) = \frac{1}{4}\frac{q^2\vec{E}^2(\vec{r})}{m\omega_{rf}^2}, \tag{1}$$

where $\vec{E}(\vec{r})$ is the numerically calculated amplitude of the time-varying electric field. The accuracy of the simulation is limited by two factors: How accurately the electrodes are represented by the Cartesian grid underlying the simulation and by the imposed convergence criteria are for the potential defined on that grid. We estimate the accuracy of the simulation for a given grid to be less than 1 meV. The accuracy due to the grid representation, however, is estimated to be about 10 meV. On top of these errors, there is a contribution from the accuracy and stability of the voltages applied to the electrodes in the experiment, which we estimate to be about 1 meV.

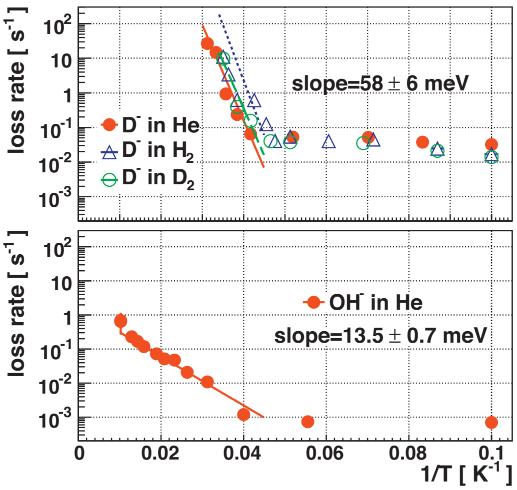

Fig. 2. The loss rate of D^- (upper panel) and OH^- (bottom panel) for varying temperature and density (upper panel only) of the buffer gas. The lines show exponential fits to the experimental data. The upper figure shows three lines for different buffer gases: red solid (He), green dashed (D_2) and blue dotted (H_2). For these three fits the average slope is indicated.

3. Experimental results

3.1. Temperature dependent losses

In this section, we present ion loss measurements as a function of the buffer gas temperature. In Fig. 2, evaporative ion loss measurements for D^- and OH^- anions are shown. We observe that the loss rate depends strongly on the inverse trap temperature down to the region of 20–25 K, where the decrease of the loss rate suddenly terminates.

We first consider the temperature regime above 25 K. Here the curves for both ions show an Arrhenius type behaviour:

$$k(T) \propto e^{-(E_a/k_BT)}, \tag{2}$$

where $k(T)$ is the loss rate of the ions, T is the temperature of the buffer gas and k_B is the Boltzmann constant. E_a is an activation energy and represents the kinetic energy an ion needs to overcome the effective trapping potential. By fitting the experimental data according to Eq. (2), we obtain activation energies for D^- of 58 ± 6meV (see Fig. 2 for details) and for OH^- of 14 ± 1 meV. This is carried out under the assumption that the ion translational temperature corresponds roughly to the temperature of the buffer gas. It will be shown in Section 3.2.2 that this assumption does not fully hold for the present experiments, which needs to be considered in a quantitative analysis as discussed below.

In the following it is necessary to distinguish ion losses in the radial direction from those along the axial directions of the trap. The activation energy is then attributed to the apparent potential barrier height in the corresponding direction. It has previously been shown [14,16] that ion losses in the radial direction are driven by non-adiabatic motion of the fast ions in the rf field and a maximum stability parameter for the adiabatic region of $\eta_{max} = 0.36 \pm 0.02$ was derived [14]. According to [7] the trapping conditions can