



Digital and Ion Trap Simulations for Heavy Biomolecule Circumstances in Ion Filter

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DESCRIPTION

In order to examine biomolecules using single-particle imaging with X-ray pulses, ion trajectories for an assembly containing a linear quadrupole ion-filter and a linear Paul trap with additional pin electrodes have been calculated. Digital guiding and trapping fields are the foundation of the ion-optical components. The module proposed consists of separate components for filtering and accumulation or trapping to select the ions of interest and to convert the beam from a continuous ion source to ion bunches as required for the experiments downstream. This allows for the careful handling of biomolecules over a broad mass-over-charge range. Mass Spectrometry for Single Particle Imaging of Cancer is the second module of the beam line, where the ions from the source region are selected, aggregated, heated up and discharged as a clearly defined ion lot for additional research.

This module is made up of a quadrupole ion filter, a linear quadrupole ion trap and linear hexa pole and quadrupole ion guides. After an analysis of digital Radio Frequency (RF) fields, section three of the document contains details of the components. The module is anticipated to handle and separate ions with a mass resolving power R on the order of 100 and several thousand Thomson ions. The radial phase space of the outgoing ion bunch must also be small enough to allow for a sequence of 2-mm openings downstream. To enable time of flight conformation separation at the ion mobility cell and to have a high-density ion bunch in the interaction region of the X-ray beam and its temporal width must be less than 100 ns. There are two rules that must be followed in order to maintain the proteins' native structure. Changing the stability conditions for the stored particles or scanning the trap frequency, is how ion selection is carried out in the majority of applications with a digital ion trap. Ion it also helps the analysis in the event of collision-induced dissociation during trapping and ejection processes. This prevents space charge effects while filtering a fully loaded trap. The ion optics simulation programme is used to calculate the electric fields and ion trajectories on a grid mesh

with a spatial resolution. For calculating ion trajectories in electric fields, a popular application is utilized. It has a lot of features and supports third party extensions. The computation time steps of the ion paths have been carefully chosen to be less than at least one tenth of the highest RF-frequency. The "transmission mode" in which the ions are led through, the "accumulation mode," where the ions are gathered, compacted together and heated in the "ejection mode" in which the collected ions are discharged are the three possible configurations for the trap. The three modes' applied voltages the potential of the entry-side end cap must be below the axial kinetic energy of the ions in the "accumulation mode" for them to enter the trap. Ions cannot enter the downstream hexa pole due to the potential of the exit-side. The pressure of the buffer gas is a crucial variable for the operation of the ion trap in addition to the possible configuration of the accumulation mode. Because the ions have distinct phase spaces for various filter settings at the entry of the trap, the trapping effectiveness is somewhat dependent on the filter conditions.

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