Collision/Reaction cell for ICP-MS - a new concept for an improved removal of low masses

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Overview

Purpose: To provide an explanation of some of the advanced technologies especially the low mass cut off properties of the QCell™ of the new Thermo Scientific iCAP Q™ ICP-MS system.

Methods: A series of examples are described that, after explanation of the working principle, showcase the use of the advanced features in the iCAP Q's QCell™ in both routine and research ICP-MS applications.

Results: Through the application of innovative technologies in the QCell™, low mass cut off properties together with Kinetic Energy Discrimination are shown to be effective for the suppression of polyatomic spectral interferences in challenging sample matrices. Additional examples of the utility afforded by the QCell™ in reactive and collisional focusing operation applications are described.

Introduction

Polyatomic interference, one of the fundamental challenges in ICP-Q-MS, can be suppressed with the use of a collision/reaction cell. Although a single gas mixture is suitable for most routine applications, some analytes in more challenging matrices benefit from an alternative (reactive) gas or more aggressive cell conditions to suppress or remove any polyatomic interferences. In reactive mode it is also important to remove the reacting gas ions and other low mass ions along the cell.

A new collision cell design employing curved flatapole rods was developed. The design combines a high transmission due to the larger r_0 at the cell entrance with a low mass cut-off at the lower r_0 in the middle of the cell. The underlying principle is the variation of q along the collision cell. This unique design combines the use of the same RF amplitude for high sensitivity and robustness as well as sufficiently high low-mass cut-off to ensure elimination of any reaction products.

FIGURE 1. Thermo Scientific iCAP Q™ ICP-MS

QCell Technology

In low mass resolution ICP-MS multipoles are used as ion guides in collision/reaction cells to suppress interferences. In contrast to higher multipoles, the quadrupole has a well-defined stability boundary that allow the removal of lower masses before they can react further down the cell (a "low mass cut-off").

In the QCell™ of the iCAP Q™ ICP-MS, a flatapole is used. This allows for a smaller cell volume compared to e.g. the one of a hexapole with a similar distance between the rods. The properties of a flatapole are very similar to that of a quadrupole. As can be seen from Figure 2 , the electric field corresponds to a quadrupole with higher multipole components.

FIGURE 2: Electric field of Flatapole (left) and Quadrupole.

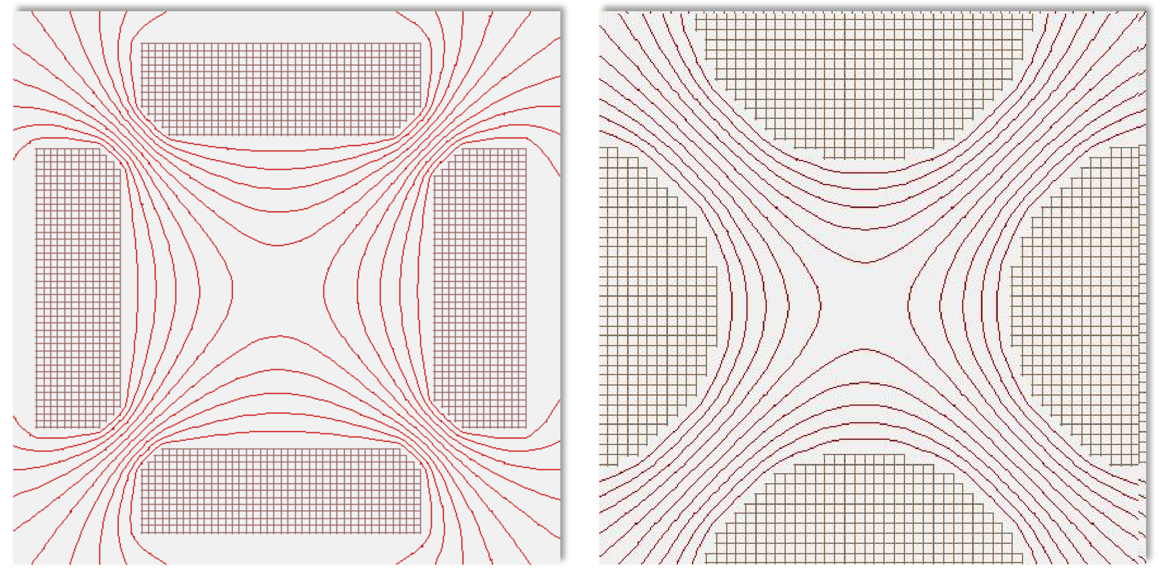
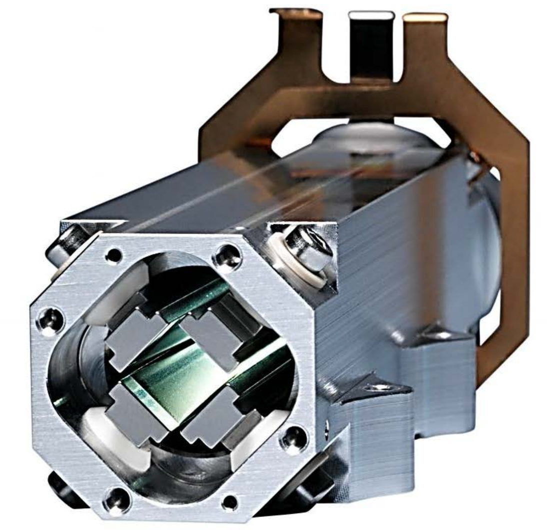


FIGURE 3: QCell™ with flatapoles



The ability of an ion to be transmitted through a quadrupole is dependent on the parameters **a** and **q** and whether the ion is within the quadrupole's stability region.

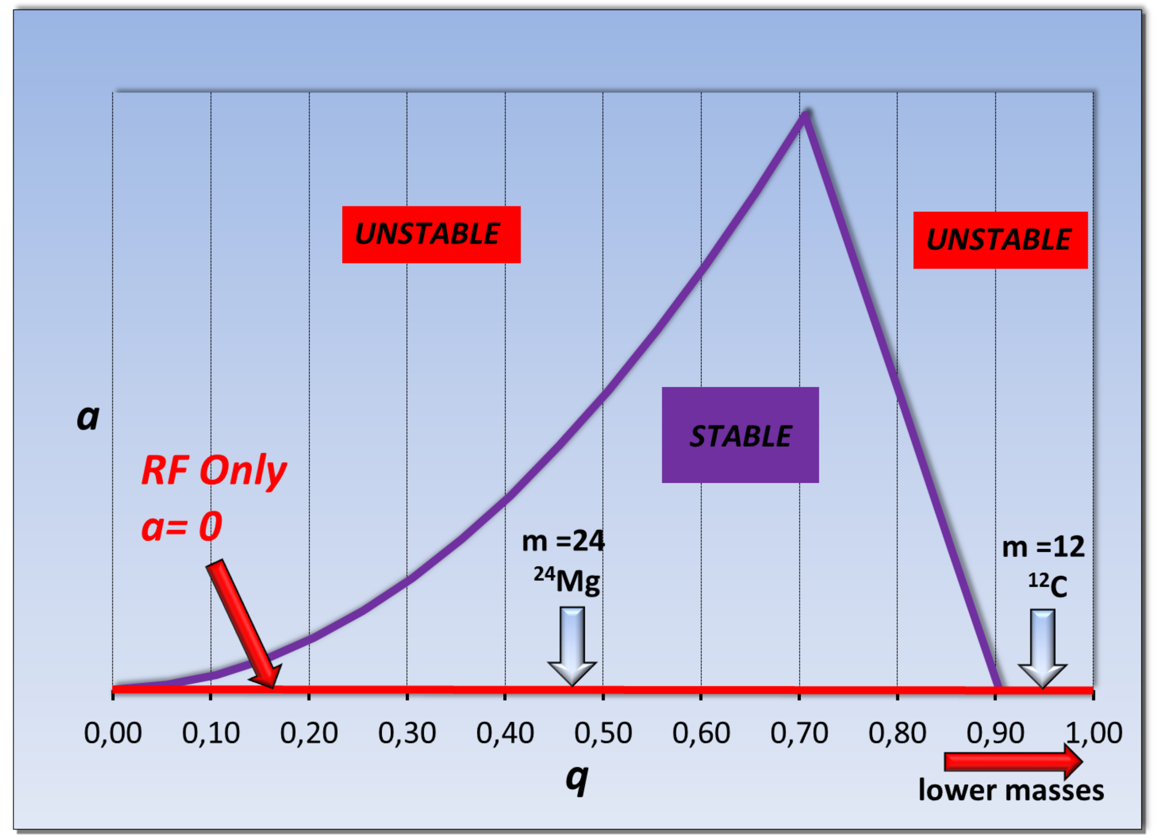
The parameter **a** (the y-axis in Figure 4) is dependent on the DC voltage applied to the rods. In RF only operation as used in the QCell™ this value is 0. The parameter **q** (the x-axis in Figure 4) is defined as:

$$q = \frac{4 \cdot e \cdot V}{m \cdot \omega^2 \cdot r_0^2}$$

As can be seen from this equation, the lower the mass, **m**, the higher the **q** value. If the **q** value exceeds the boundary of the stability region, this mass and all masses below it are unstable and are removed within the cell: the low mass cut-off effect.

The equation also shows that the shorter the distance between the rods (r_0), the higher the **q** value. This means that for two quadrupole systems with different rod separations, a low mass cut off will be achieved at higher masses for the smaller r_0 values system.

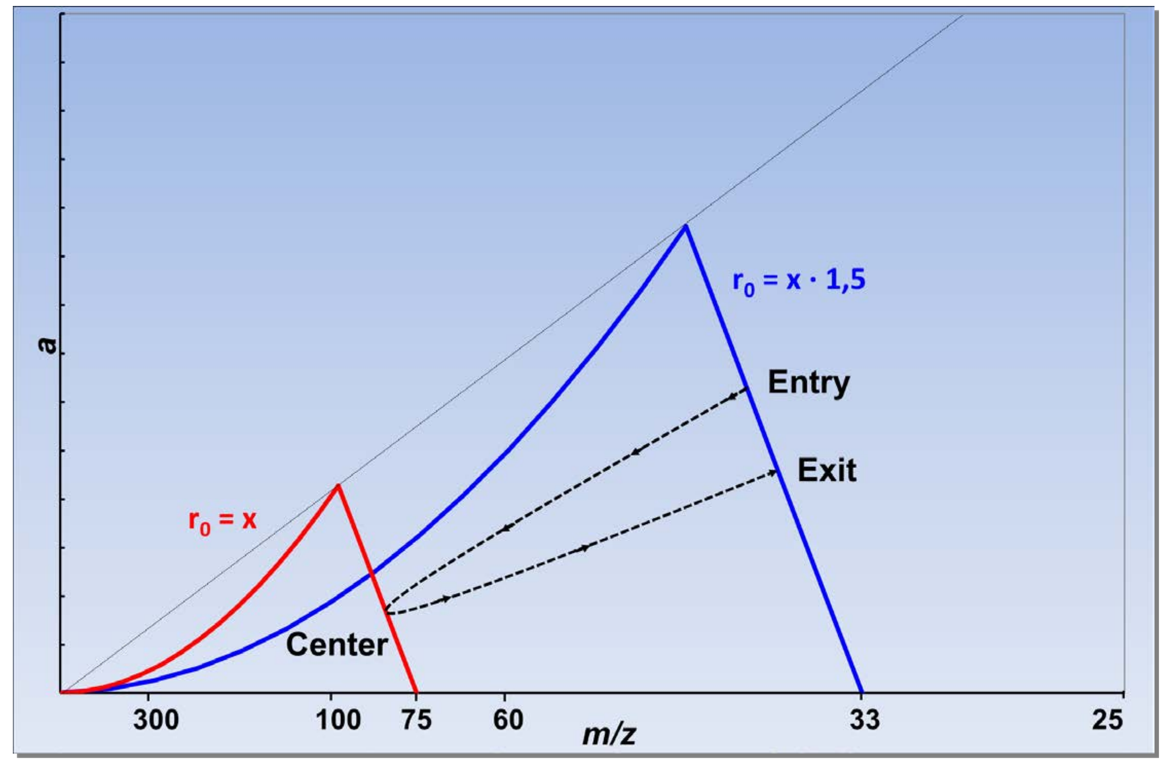
FIGURE 4: Example Stability diagram of a quadrupole.



The QCell™ has curved shaped flatapole rods so that the distance between the rods (r_0) decreases from the entrance to the center of the cell and increases again towards its end. Therefore, the stability region changes with distance from the cell entry. In operation, the upper boundary of stability remains constant at q = 0.905, but this boundary moves along the mass scale along with the axial distance through the curved quadrupole.

In Figure 5 the stability plots for 2 different r_0 are displayed. In this example the "larger" stability plot is for the distance r_0 which is 50% larger than for the second, smaller stability plot. At the entrance of the QCell™ to the curved flatapole, the boundary is given by the first stability plot for r_0 = 1.5 x. With further penetration into the QCell™ towards its center, the stability plot shrinks on the mass scale - so the boundary moves - to the second stability plot for r_0 = x. Upon passing the center of the flatapole and passing further downstream towards its end, the stability plot expands again on the mass scale - so the boundary again moves – back to the first stability plot for r_0 = 1.5 x. Another way of describing this example is to say that, for a given mass, the q value starts at a relatively low value at the entrance to the flatapole and grows by a factor of 2.25 towards the center [$q2/q1 = (1.5\ x)^2/(x)^2$] and then shrinks again to its initial lower value towards the downstream end.

FIGURE 5: Stability diagram for curved rods.



Results

He KED Analysis with the iCAP Q™ ICP-MS

As an example of the power of He KED mode for the removal of background and matrix induced polyatomic interferences in ICP-MS, a series of mass spectra were acquired.

FIGURE 6. iCAP Q™ He KED 5% HNO_3 Blank.

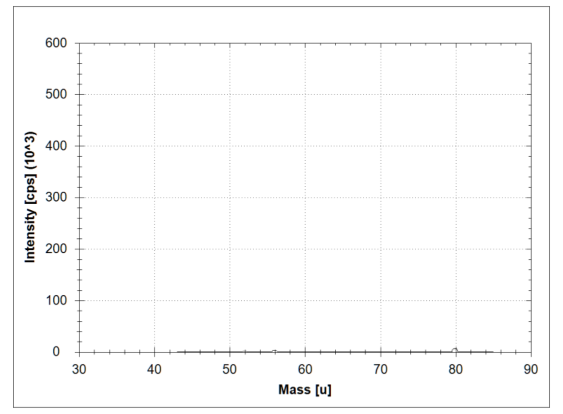
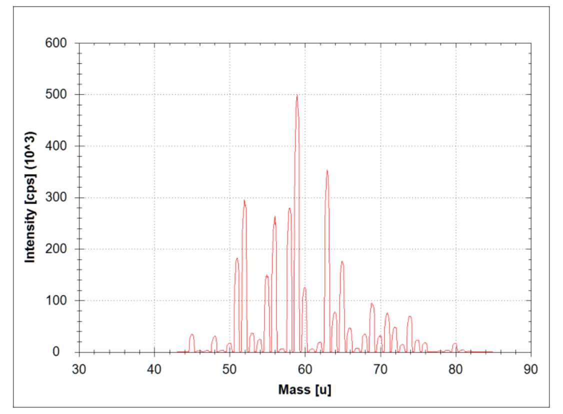


FIGURE 7. iCAP Q™ He KED 5% HNO_3 Blank + 10ppb multi-element spike.



Figures 6 and 7 show the mass spectra for a simple 5% HNO_3 blank and the same mass range for the same solution spiked with a range of transition row elements.

FIGURE 8. iCAP Q™ He KED 5% HNO_3 5% HCL 1% IPA 1% H_2SO_4 Blank

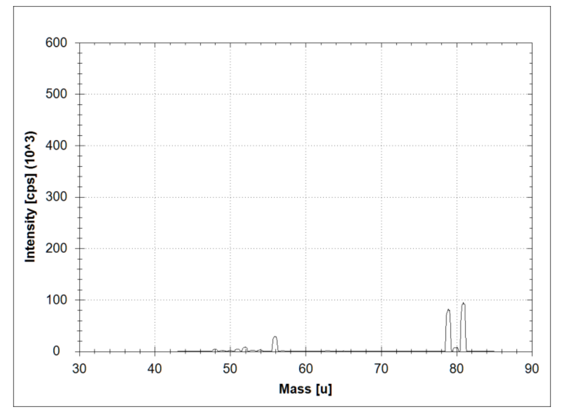
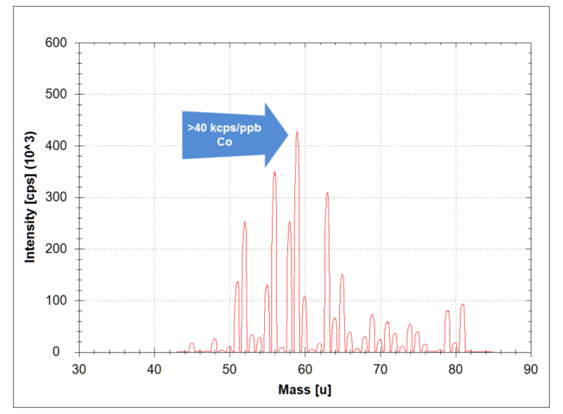


FIGURE 9. iCAP Q™ He KED 5% HNO_3 5% HCL 1% IPA 1% H_2SO_4 Blank + 10ppb multi-element spike



Figures 8 and 9 show the mass spectra for a 5% HNO_3 5% HCL 1% IPA 1% H_2SO_4 Blank and the same mass range for the same solution spiked with a range of transition row elements. Apart from Br contamination (from the HCl) at m/z 79 and 81 there is little difference between Figures 7 and 9.

FIGURE 10. iCAP Q™ He KED 5% HNO_3 5% HCl 1% IPA 1% H_2SO_4 200ppm Na 500ppm P 200ppm Ca Blank

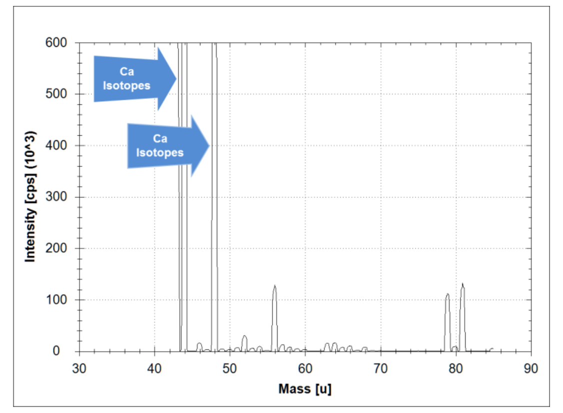
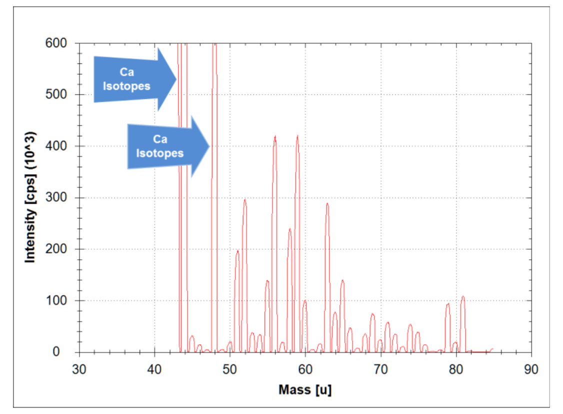


FIGURE 11. iCAP Q™ He KED 5% HNO_3 5% HCl 1% IPA 1% H_2SO_4 200ppm Na 500ppm P 200ppm Ca Blank + 10ppb multi-element spike



Figures 10 and 11 show the mass spectra for a 5% HNO_3 5% HCL 1% IPA 1% H_2SO_4 200ppm Na 500ppm P 200ppm Ca Blank and the same mass range for the same solution spiked with a range of transition row elements. Even in this most complicated He mode, KED on the iCAP Q™ provides comprehensive reduction of interferences.

Improving ICP-MS Performance with Reactive Chemistry

The QCell™ can also be operated in a purely reactive CCT mode without any KED barrier. For Se for example, by pressurizing the QCell™ with a safe 7% H_2/He mixture, improved performance can be achieved since the highly reactive H_2 efficiently removes the Ar based interferences that limit its analysis in many application areas.

FIGURE 12. iCAP Q™ 7% H_2/He CCT Calibration for ^{78}Se

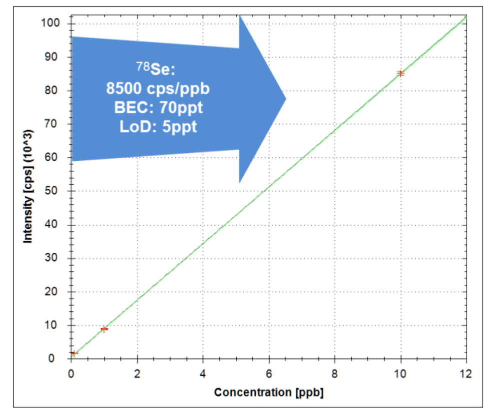
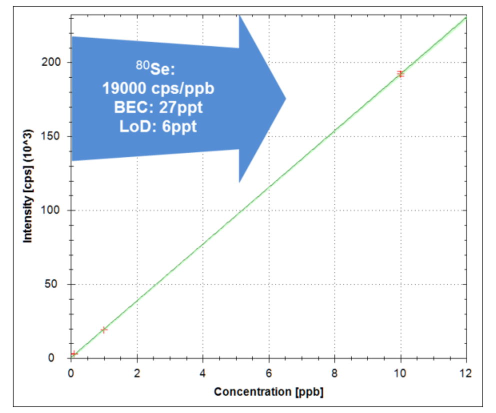


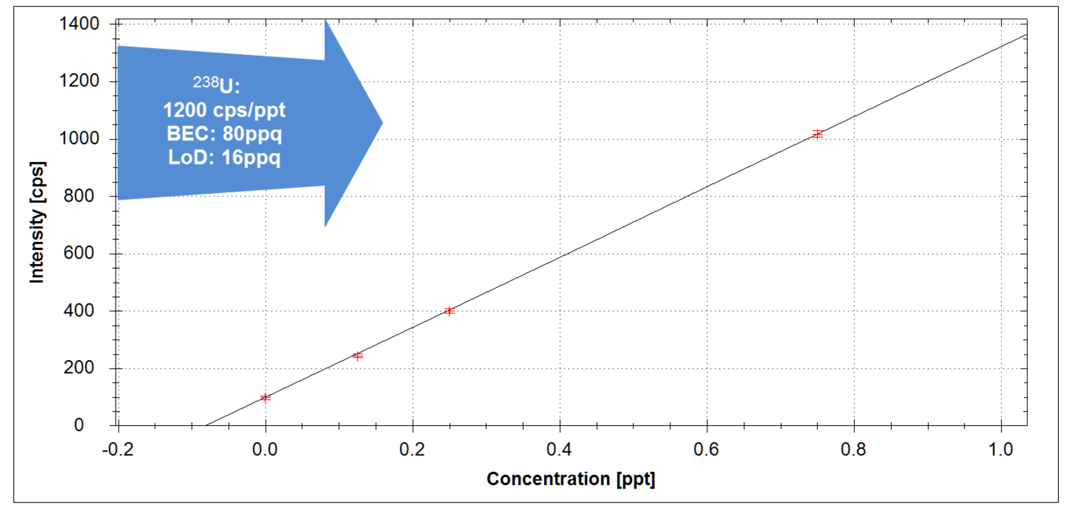
FIGURE 13. iCAP Q™ 7% H_2/He CCT Calibration for ^{80}Se



Improving ICP-MS Performance by Collisional Focusing

The iCAP Q™ QCell™ can also be operated without a KED barrier. In this mode, collisional focusing / dampening processes occur that allow – for example – for improved sensitivities when using pure He as the CCT gas.

FIGURE 14. Screenshot from the Qtegra control software showing a sub-ppt ^{238}U calibration. With instrumental sensitivities of >10^6 cps per ppb, detection limits (LoD) and background equivalent concentrations (BECs) comparable to Sector Field ICP-MS instruments are achievable.



Conclusions

- The new QCell™ technologies introduced in the iCAP Q™ with its Flatapole and Low Mass Cut-off provide the end user with significant improvements in the routine use of kinetic energy discrimination (KED) for interference removal in ICP-MS analysis
- The curved flatapole rods offer an enhanced low mass cut-off that provides the Analytical Chemist a wide range of possibilities for flexible uses of reaction and collision cell approaches in challenging applications and fundamental research.

Acknowledgements

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