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iCAP TQ ICP-MS

SmartNotes

QA

Triple Quadrupole ICP-MS or Single Quadrupole ICP-MS? Which Instrument is Right for Me?

What is a triple quadrupole ICP-MS?

The IUPAC definition of a triple quadrupole mass spectrometer is a *'tandem mass spectrometer* comprising two *transmission quadrupole mass spectrometers* in series, with a (non-selecting) *RF-only quadrupole* (or other multipole) between them to act as a *collision cell'*[1]. In ICP-MS, the three quadrupoles, Q1, Q2, and Q3 are in a linear arrangement between the inductively coupled plasma (ICP) and the detector. The two quadrupoles Q1 and Q3 are mass filters and the Q2 quadrupole is a collision/reaction cell (CRC).

How is a triple quadrupole different from a single quadrupole ICP-MS?

A single quadrupole (SQ) is typically an arrangement of a mass filtering quadrupole and a CRC. When compared to a triple quadrupole, both systems have a CRC (highlighted in blue in Figure 1) and an analyzing quadrupole (highlighted in green in Figure 1). The triple quadrupole, in comparison, has an additional quadrupole (highlighted in yellow in Figure 1) situated prior to the CRC.

SQ-ICP-MS provides comprehensive interference removal with helium gas and kinetic energy discrimination (SQ-KED) adequate for many trace elemental analyses. However, a SQ can have limited success in the analysis of certain analytes in matrices where specific interferences cannot be removed by SQ-KED. This is where the additional quadrupole and improved interference removal with a TQ system can make the difference.

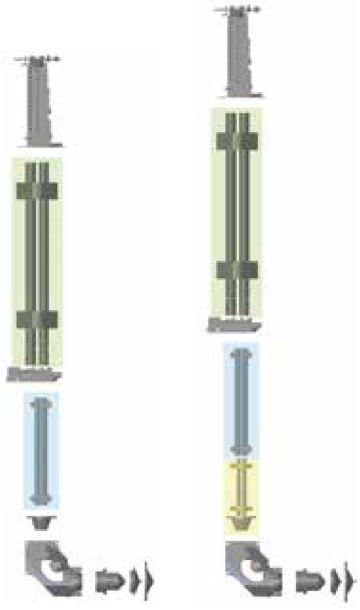

Figure 1. Left.) Single Quadrupole ICP-MS and Right.) Triple Quadrupole ICP-MS.

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Are all three quadrupoles in a triple quadrupole ICP-MS exactly the same?

No, they are not all the same. The two quadrupoles Q1 and Q3 are mass filters and the Q2 quadrupole is a CRC.

How does a mass filter differ from a collision/reaction cell?

A quadrupole mass filter means that we apply both DC and RF voltages to the quadrupole to create a specific mass stability range and selectively filter masses of interest. Other masses, that are not stable at the particular DC and RF setting are ejected from the ion beam, collide with the rods and eliminated from any further processes in the system. A CRC typically uses only an RF field to control the trajectory of ions through this component and does not apply a specific mass filter.

What are the functions of the three quadrupoles?

Q1: The first quadrupole acts as a first mass filter which selectively transmits ions into the second quadrupole. The benefit of this first quadrupole is that far fewer low mass precursor ions (such as H, C, N and O) enter the second quadrupole. These precursor ions arise as a result of the components present in the sample matrix and the instrument plasma, which is running at atmospheric pressure. Removing them eliminates the chance for them to enter the second quadrupole and generate additional interferences. This means that the cell is more efficient in removing interferences coming directly from the plasma and sample. In the case of TQ reactive mode, this selective transmission allows more controlled reactions to be carried out on the target isotope in Q2.

Q2: The second quadrupole acts as the collision/reaction cell of the instrument. This quadrupole can be used either in conventional collision mode, using pure He as the cell gas, or in reactive mode, using reactive gases. In collision mode, the instrument operates in much the same way as a single quadrupole ICP-MS. In reactive mode, gases such as ammonia (NH_3) are used to perform selective reaction chemistry on either the target isotope or on the interference(s) to create a specific product ion. These on-mass or mass-shift product ions are then transmitted to the third quadrupole.

Q3: The third quadrupole acts as both the second mass filter and the analyzer quadrupole in the ion flight path. Due to the selective reactions in Q2, the product ions of the target analyte have a different mass compared to the interfering ions and, as such, are filtered by the third quadrupole for detection.

What is the benefit of having three quadrupoles for interference removal?

The power of this approach comes from the ability to use three quadrupoles to filter ions of a certain mass, both before and after passing through the collision/reaction cell. This is particularly advantageous for using the second quadrupole as a reaction cell where gas-phase reaction chemistry can be used to shift either the mass of the interference (e.g. removing ^{40}Ar interference on ^{40}Ca using H_2 reaction gas) or that of the target analyte (e.g. measuring ^{32}S at mass 48 after reaction with oxygen (O_2) to form SO^+ which is free from the $^{16}O_2^+$ interference). Only the mass of interest is then transmitted through the third quadrupole.

This approach facilitates lower detection limits than those that can be achieved with single quadrupole ICP-MS instruments (even if they are operated in reactive mode) and is ideal for difficult applications such as trace Ti determination in biological fluids for research purposes, as shown in Figure 2.

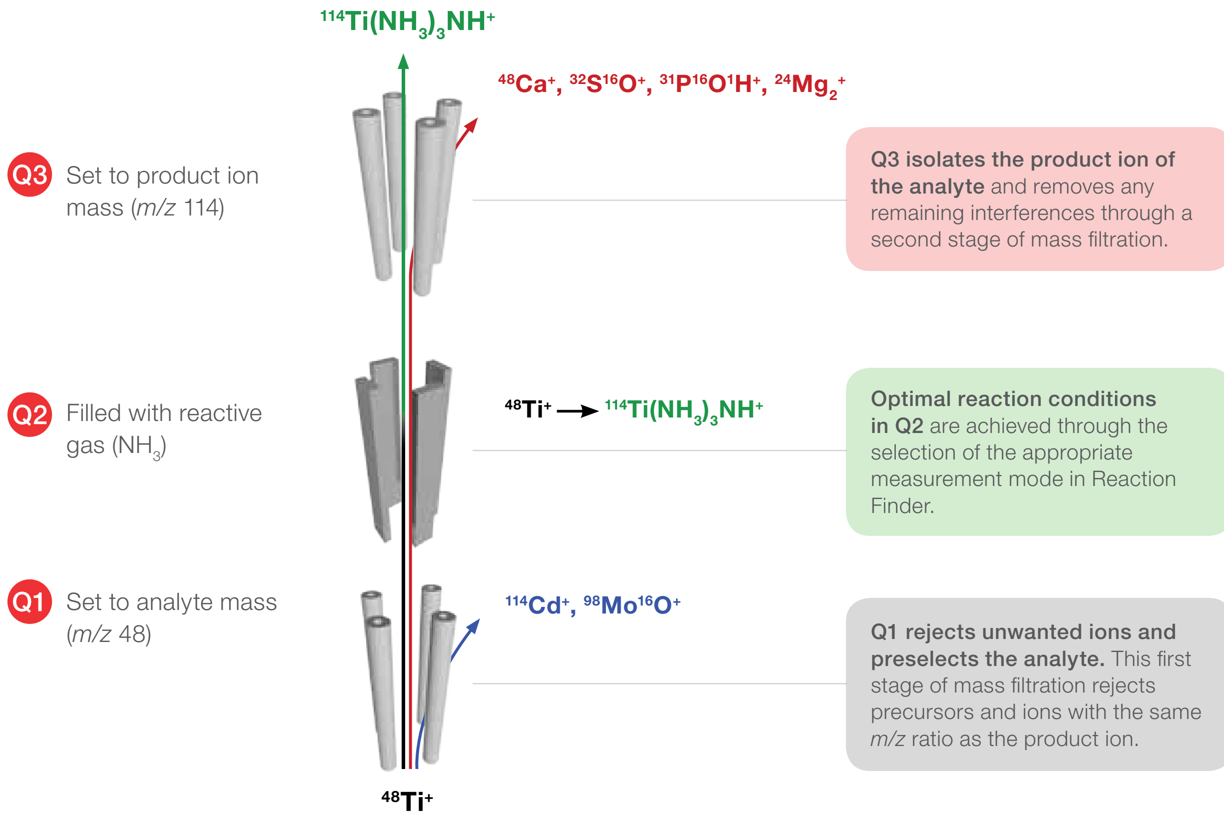

Figure 2. TQ mass shift mode for Titanium.

What range of collision/reaction cell gases can be used with the triple quadrupole instrument?

In principle, any gas that does not damage the hardware of the instrument can be used. In practice, the most common gases that are used include He (collision gas) and NH_3, O_2 and hydrogen (H_2) (reaction gases). As all of these gases can be used in a single method, the best limits of detection can be achieved for nearly all analytes and matrices in one analytical run.

TQ-ICP-MS instruments use hazardous cell gases, therefore what safety precautions are required?

The required safety features include a valve-restriction module for the cell gas supplies and a pressure sensor for monitoring the instrument exhaust flow. These safety features are built-in as standard into every system prior to shipment to ensure safe operation in every lab.

Which instrument type should I choose: a single or triple quadrupole ICP-MS?

The choice depends on what your analysis requirements are. For example, if you analyze drinking water in accordance with regulatory levels for a range of elements, then a single quadrupole ICP-MS is likely to meet your requirements. If you work in a contract analysis laboratory, where typically a number of different sample types are measured, a single quadrupole instrument will generally be suitable. However, there may be some specific analytical challenges (such as low level Se analysis in soil samples, where interference from doubly charged rare earth elements can be a problem) that require triple quad technology. If your laboratory needs to perform more complex analyses, such as trace element measurement in metal / metal alloy solutions, or Ti distribution in biological fluids for research purposes, the interference removal capabilities of a triple quadrupole instrument will be beneficial to you. For academic research laboratories, the flexibility and extended capabilities of a triple quadrupole instrument allow the widest possible range of elemental analysis research applications.

Can a triple quad ICP-MS be used in single quad mode for routine applications?

Yes, by setting the first quadrupole to operate as just an ion guide, the instrument is made to behave exactly like a single quadrupole instrument. All of the measurement modes available on a single quadrupole instrument can be used on a TQ-ICP-MS. It is also possible to switch between triple quadrupole mode and single quadrupole mode during a single analysis, allowing complete, optimised measurements of the each sample in the same analytical run.

Is a TQ-ICP-MS better for handling samples with complex matrix?

This answer is dependent on the specific components in the matrix. If you have samples with high levels of dissolved solids, then as a general rule, any ICP-MS system can easily tolerate up to 0.2% of total dissolved solids (TDS). If higher matrix loads are expected in the sample, the use of autodilution or Argon Gas Dilution (AGD) is a way to overcome potential issues caused by the matrix. If, however, you have samples with a mixture of elements that generate a wide variety of spectral interferences in the plasma, then a triple quadrupole ICP-MS can be better than a single quadrupole instrument, when it comes to getting more accurate results and fewer false positives.

How difficult is it to learn TQ-ICP-MS in comparison to SQ-ICP-MS?

This depends on which method development features are available in the instrument's software.

While it is true that without pre-configured, method development templates, triple quadrupole instruments are more complex to operate (due to the extra reactive gases that are available for interference removal and the extra Q1 settings) with the right software tools these instruments are as straightforward to operate as single quadrupoles. The Thermo Scientific™ Qtegra™ Intelligent Scientific Data Solution™ (ISDS) Software provides integrated tools such as Reaction Finder (which includes pre-tested default settings for all possible reactions with a range of cell gases) and pre-optimized measurement modes so that operation is greatly simplified. The stepwise workflow of getting a TQ-ICP-MS instrument set up and ready for analysis can, therefore, be almost as simple as that for a SQ-ICP-MS. In this case, learning to operate the TQ-ICP-MS becomes straightforward.

Routine maintenance and sample introduction configuration is the same on both instrument types, so there is no additional complexity in these areas.

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How can Qtegra ISDS Software help with TQ-ICP-MS analysis?

Qtegra ISDS Software assists the user with instrument start up and performance verification using our integrated 'Get Ready' process. This process controls plasma ignition and performance checking against previously specified criteria. Autotuning, if required, is performed automatically to ensure optimum performance of the instrument before starting your analysis. All information and reports relating to these steps is automatically stored for audit trail purposes. Qtegra ISDS Software also allows manual interaction with the instrument tune settings, should the user wish to make any manual adjustments.

Next, Reaction Finder assists with providing factory-tested, pre-defined settings for a range of cell gases with a broad range of elements. This means that the user need only select the elements of interest during method set up. No laborious optimization of the cell gas or evaluation of different cell gases is required, as all of this method development has been done for you and stored in the pre-defined settings described above. As you work through the workflow and select your analytes, the software will display suitable measurement modes based on the gases that are connected to the instrument. This can be the single quadrupole modes you already use or the appropriate TQ mode. Based on your selection, the software will suggest the appropriate settings for the analysis so that the LabBook is ready to run within minutes.

In addition, there is no need to optimize all the different TQ modes each time you use them. The pre-defined measurement modes mean that, day to day, you need only optimize the instrument conditions for the plasma source and interface region (e.g. nebulizer gas flow, torch position, extraction lens voltage) and the parameters are applied to all the relevant measurement modes. For additional ease of use, the Get Ready process can do that all automatically for you.

References

1. IUPAC Standard Definitions of Terms Relating to Mass Spectrometry; K.Murray and co., Pure Appl. Chem., 2013, Vol. 85, No. 7, pp. 1515-1609

Find out more at **thermofisher.com/TQ-ICP-MS**

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