SmartNotes

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

When analyzing challenging samples, interferences can be a major source of uncertainty in ultra-trace determination of a wide range of elements. Strategies to reduce interferences on these analytes either involve using collision/reaction cells in quadrupole instrumentation to physically or chemically alter the ion beam in a controlled manner to isolate the analyte from the interference, or use high resolution instrumentation to discriminate the analyte next to an interference with a high degree of accuracy.

With the addition of the Thermo Scientific™ iCAP™ TQ ICP-MS to the Thermo Scientific portfolio of ICP-MS instruments, we now offer a comprehensive range of ICP-MS instrumentation to cover all of your trace and ultra-trace analytical needs. While it is clear that triple quadrupole (TQ) ICP-MS offers benefits over single quadrupole (SQ) instruments, it is perhaps less obvious if high resolution (HR) ICP-MS is a more suitable technique than TQ-ICP-MS for certain analysis. This Smart Note will clarify when TQ-ICP-MS or HR-ICP-MS would be the better option for a particular analysis.

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How does a triple quadrupole ICP-MS work?

Triple quadrupole ICP-MS allows a single mass or narrow range of masses to be selected by the first quadrupole (Q1), prior to the ion beam entering the second quadrupole. The second quadrupole (Q2) is a collision/reaction cell (CRC), which can be operated with a variety of different cell gases. This enables a broad range of chemical reactions (or collisions when pure He is used as the cell gas) to be carried out for specific interference removal. The third quadrupole (Q3) is then used to isolate the analyte from the interference for measurement.

Interference removal based on reactions in Q2, fall into two groups, TQ on mass mode and TQ mass shift mode. In TQ on mass mode, the analyte isotope is measured on-mass after chemical reaction to remove the overlapping interference (e.g removal of $^{40}Ar^{+}$ on $^{40}Ca^{+}$ using H_2 as a reactive cell gas). In TQ mass shift mode, the analyte isotope interacts with the reaction gas to produce a product ion that is free from the original interference (e.g. removal of $^{48}Ca^{+}$, $^{31}P^{17}O^{+}$ and $^{31}P^{16}O^{1}H^{+}$ interference on $^{48}Ti^{+}$ by reaction with NH_3 cell gas to produce $^{114}Ti(NH_3)_3NH^{+}$).

As with single quadrupole ICP-MS instruments, TQ-ICP-MS typically provides unit mass resolution for routine operation, which means that the resolution of the masses transmitted to the detector is one mass unit across the whole mass range. So, for example, mass 77 can be resolved from mass 78 but mass 77.5 is not distinct from mass 78. The resolution can be increased slightly so that separation of mass 77.5 from 78 can be improved but this is limited in practice to around 0.3 mass unit resolution, and results in significant loss of sensitivity. This mass resolution is insufficient to separate common interferences from an analyte, such as $^{40}Ar^{16}O^{+}$ from $^{56}Fe^{+}$.

How does a high resolution, magnetic sector ICP-MS work?

High resolution, magnetic sector ICP-MS uses a magnetic field to steer ions generated by the plasma through a curved path to the detector. The extent to which the ion trajectory curves as it passes through the magnet depends mainly on the mass to charge ratio of the ion and the strength of the magnetic field provided by the magnet. Apart from the differences in hardware, the most fundamental difference between quadrupole and magnetic sector ICP-MS instruments is their mass resolution capability. While quadrupole based instruments have unit mass resolution, so transmit one mass unit at a time to the detector, magnetic sector instruments can provide up to 10,000 mass resolution. Since mass resolution is defined as $\frac{m}{\Delta m}$ at a 10% valley between peaks[1], this equates to resolving peaks separated by just 0.005 mass units at low masses.

This high resolution is achieved by combining the magnet with an electrostatic analyzer, which focuses the ions according to their energy spread, and a pair of physical slits that define the peak profiles at the detector. What this means in practice is that HR-ICP-MS is capable of completely resolving, for example, $^{56}Fe^{+}$ (55.935 u) from $^{40}Ar^{16}O^{+}$ (55.957 u). HR-ICP-MS instruments do not use collision cell technology for reducing or removing interferences. Just as any other technique, a higher resolution means in turn a lower signal, so that in practice highest mass resolution is just used for the separation of the most complicated interferences. Lower resolution settings (but still higher resolution when compared to quadrupole ICP-MS) are often preferred when less demanding interferences have to be handled, for example resolving $^{47}Ti^{+}$ against a host of polyatomic interferences (Figure 1).

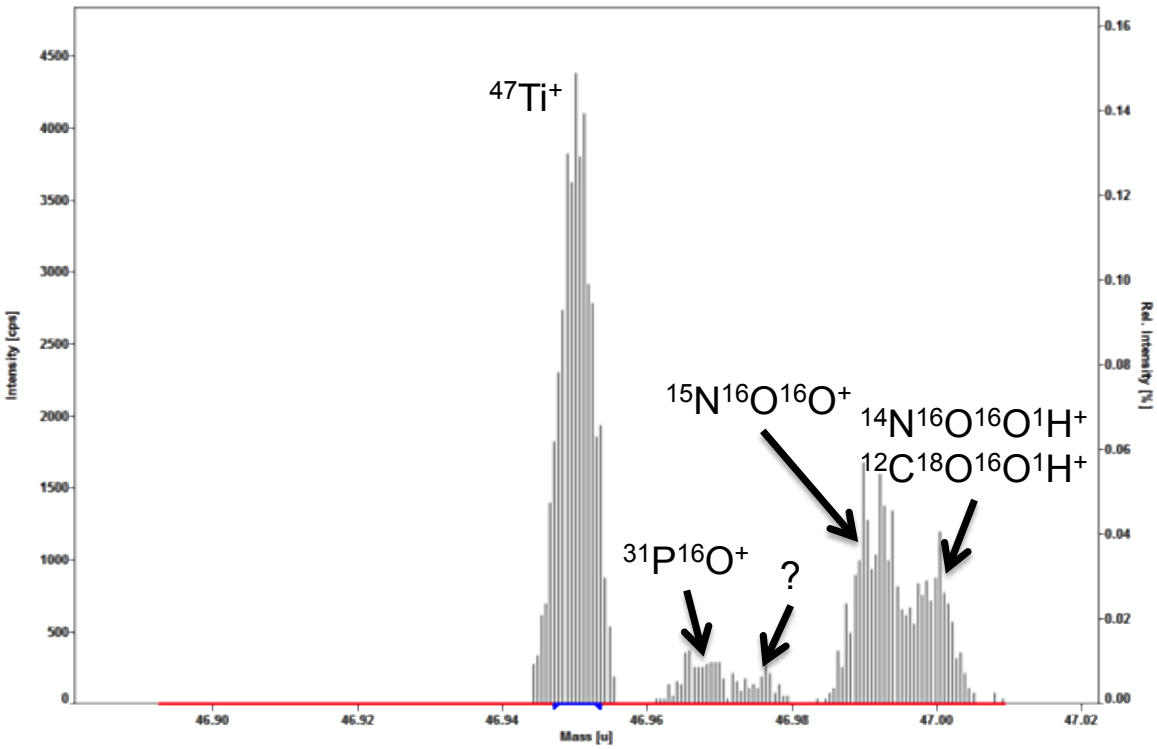

Figure 1. $^{47}Ti^+$ **resolved from polyatomic interferences at medium resolution (**$\frac{m}{\Delta m}$ **= 4000) using a HR-ICP-MS.**

Why would I choose TQ-ICP-MS if HR-ICP-MS can solve my interference problems?

As powerful as high resolution ICP-MS is, there are some interferences that it cannot resolve because they require mass resolving powers greater than 10,000. Examples include some polyatomic interferences, such as MoO^+ interference on Cd^+ where the resolution required > 30,000, or better than 0.003 mass units.

Other examples include isobaric interferences (i.e. isotopes of different elements with the same mass) such as $^{64}Ni^+$ interference on $^{64}Zn^+$, or $^{90}Zr^+$ interference on $^{90}Sr^+$ usually cannot separated by their mass differences, often required 30 to 40 times better resolving power than high resolution can offer.

How can TQ-ICP-MS handle these interferences then?

TQ-ICP-MS has the benefit of being able to use chemical reactions within the collision cell of the instrument to provide solutions for interferences that require mass resolving power that is beyond the reach of HR-ICP-MS. By using O_2 as the reaction gas, in the above examples MoO^+ can be converted to MoO_2^+ (and higher Mo oxides) while Cd^+ does not react. The MoO^+ interference is then shifted to a new mass leaving Cd^+ interference free. In the same way, $^{90}Zr^+$ interference on $^{90}Sr^+$ is removed by converting $^{90}Zr^+$ to $^{106}ZrO^+$ (and $^{107}ZrOH^+$) while $^{90}Sr^+$ hardly reacts.

In that case, why would I use HR-ICP-MS then?

HR-ICP-MS is capable of resolving a very wide range of interferences reliably and predictably, so is highly effective for a range of multi-elemental applications with minimum effort for application development. In addition, most interferences can be identified visually, making it easy to choose the required resolution. It is also usually not necessary to spend much valuable time actually identifying the nature of the interfering species, as long as they are mass separated from the analytes of interest.

With isobaric interferences, it is often possible to use an alternative isotope of the element of interest, which removes that problem. HR-ICP-MS is also up to 10x more sensitive that quadrupole ICP-MS and can achieve better isotope ratio precision for key elements such as U. Improved isotope ratios are achieved by setting the magnet to one mass and applying a scanning voltage prior to the magnet to very rapidly change the mass reaching the detector (e.g. to jump from ^{235}U to ^{238}U). Ultimately, various options are available for sector field instruments to boost sensitivity by using accessories like the Jet interface, making sub ppq detection limits achievable (Figure 2).

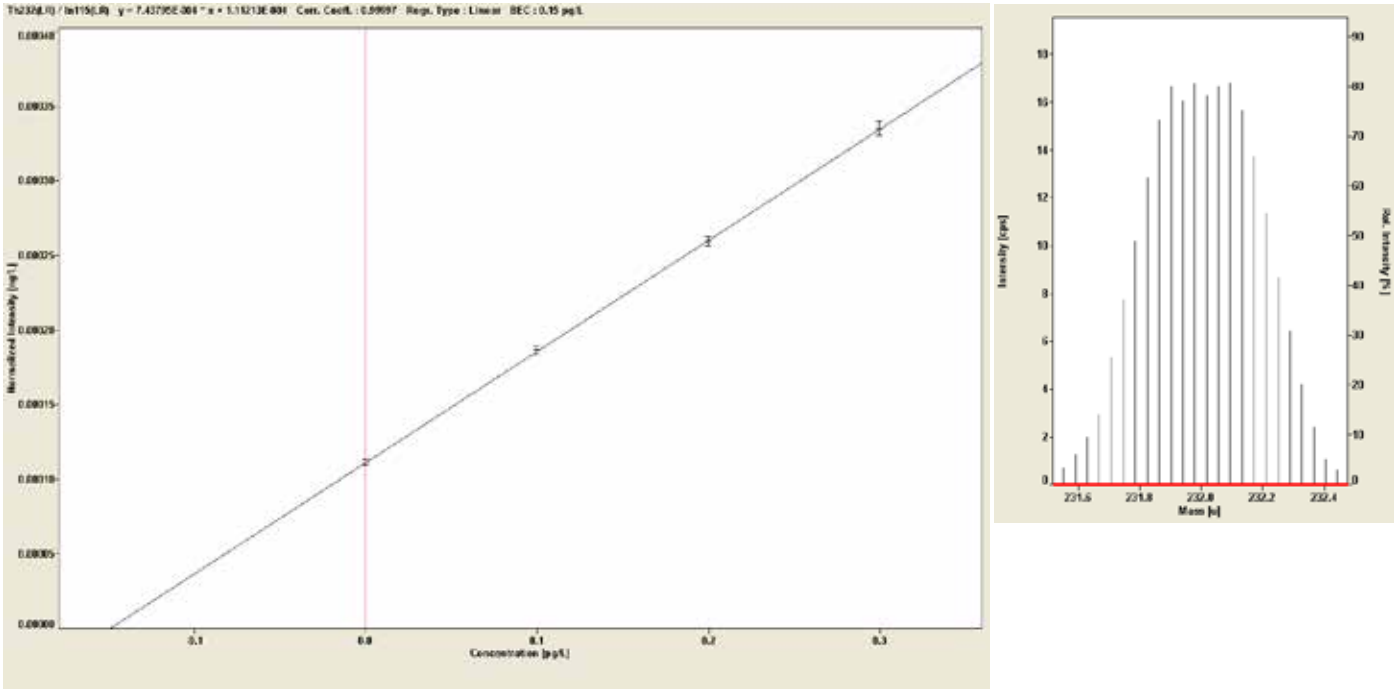

Figure 2. Standard Additions calibration of $^{232}Th^{+}$ using 0.1, 0.2 and 0.3 ppq spikes showing better than 99.99% linearity and a limit of detection of 0.005 ppq using HR-ICP-MS. Inset showing the spectra of 0.15 ppq Th.

I see where TQ-ICP-MS has advantages over HR-ICP-MS when it comes to difficult interferences and I understand where HR-ICP-MS is the better instrument, but what else should I consider?

Aside from its chemical interference removal capability, TQ-ICP-MS does have the additional advantage that it can be easily set up to run like a conventional, SQ-ICP-MS instrument. This means that, for routine applications that don't require the enhanced abilities of triple quadrupole operation, TQ-ICP-MS can simply be switched to SQ mode. This makes the instrument highly flexible for a broader range of applications.

HR-ICP-MS, on the other hand, has the distinct advantage in many cases of being able to uniquely resolve the isotope of interest so there is no doubt that what is being measured is the specific element required and nothing else. With any quadrupole technology there is always the possibility that small residual interference signals can remain, which limits the absolute accuracy that can be achieved especially in highly complex matrix samples. This makes HR-ICP-MS a very versatile technique for multi-element analysis that can use the same set of analytical settings (i.e., isotopes and resolution) for a wide variety of samples types.

As an example, the methods for running geological, environmental or food samples are virtually identical for HR-ICP-MS. Additionally, HR-ICP-MS benefits from a larger linear dynamic range detection system, which allows concentrations to be measured from sub-pg/mL levels to low % concentrations.

So which applications fit best to which of these technologies then?

HR-ICP-MS is undoubtedly the best technique for ultralow detection of non-interfered elements and for elements that require low to medium resolution (e.g. 400 to 4000). Its high sensitivity, broad unambiguous isotope identification capability and isotope ratio precision performance make it ideal for routine and research applications in semiconductor, nuclear and geological analysis. It is also well suited to clinical research applications.

TQ-ICP-MS is the best technique for routine applications that benefit from its SQ capabilities and for a very wide range of interference problems solvable using its reactive cell gas TQ abilities. Its flexibility and simplicity of operation make it ideal for routine industrial, geological, semiconductor and more challenging environmental analysis and its reactive gas cell operation provides the analytical enhancement required for clinical research applications.

So now I understand how these techniques are positioned in terms of their analytical capabilities and performance, but what about their purchase and running costs?

HR-ICP-MS is more expensive to buy than TQ-ICP-MS, being roughly 1.5x to 2x the price. In terms of installation costs, TQ-ICP-MS will be a little more expensive than HR-ICP-MS as provision needs to be made for additional gases for CRC operation. With regard to day-to-day running costs, both instruments use similar argon gas flows for the plasma, but electrical costs will be a little higher for HR-ICP-MS.

What about ease of use? Will my scientists and laboratory personnel need to have prior experience or require specialist training?

The iCAP TQ ICP-MS has been developed with simplicity of operation at the forefront of its hardware and software design. With features such as Reaction Finder in its field proven Thermo Scientific Qtegra™ Intelligent Scientific Data Solution™ (ISDS) Software, it is as straightforward to set up a reaction gas triple quadrupole analysis as it is to use a conventional SQ-ICP-MS, with only limited training.

Our HR-ICP-MS instruments, the Thermo Scientific ELEMENT™ 2 ICP-MS and Thermo Scientific ELEMENT XR™ ICP-MS, are more commonly used in research laboratories or by laboratory personnel who have prior ICP-MS experience, and in general require more training than our quadrupole instruments. That said, instrument set up and method development is straightforward with HR-ICP-MS systems, once some experience has been gained.

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I now understand how both techniques generally compare. My final question is: what about coupling accessories such as chromatography instruments or laser ablation systems with each instrument? Is this easy to do?

Yes, both HR-ICP-MS and TQ-ICP-MS can be easily coupled with chromatography and laser ablation accessories. With the iCAP TQ ICP-MS, our ChromControl Plug-in for the Qtegra ISDS Software package allows fully integrated, automated control of our full range of IC and LC systems. ChromControl Plug-in also allows control of the Thermo Scientific Trace 1310 GC, which is also supplied with a heated transfer line as part of the Thermo Scientific GCI-100 Interface for coupling to the Thermo Scientific iCAP™ Qnova Series ICP-MS. Dedicated plugins for automated control of a variety of third party laser ablation accessories are also available.

For our HR-ICP-MS instruments, all accessories can be used as well. A difference is that the coupled devices are controlled via dedicated software programs installed on the host computer. As an example, coupling of a GC system is done via the Thermo Scientific GCI-200 Interface, and Thermo Scientific Chromeleon™ Chromatography Data Solution Software can be used to both evaluate the automatically exported GC data and for control and method development of the GC.

References

1. IUPAC. Compendium of Chemical Terminology, 2nd ed. (the “Gold Book”). Compiled by A. D. McNaught and A. Wilkinson. Blackwell Scientific Publications, Oxford (1997). XML on-line corrected version: http://goldbook.iupac.org (2006-) created by M. Nic, J. Jirat, B. Kosata; updates compiled by A. Jenkins. ISBN 0-9678550-9-8. doi:10.1351/goldbook.

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