White Paper

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Exploring Four Capabilities that Are Defining the Future of ICP-MS

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Overview

Inductively coupled plasma-mass spectrometry (ICP-MS) is the most versatile tool for ultra-trace metal analysis. Today, requirements for simplified method development and more streamlined workflows are combined with the need for ever-lower detection limits and improved accuracy in the presence of complex sample matrices. These requirements drive instrument development and have resulted in the introduction of a tandem ICP-MS instrument with a triple-quadrupole (ICP-QQQ) configuration.

This executive summary describes four capabilities of a tandem MS instrument (the Agilent 8900 ICP-QQQ) that are defining the future of ICP-MS technology and offers a clear distinction between traditional ICP-MS and bandpass (BP-ICP-MS) instrumentation.

History of ICP-MS

Since the 1980s, analysts worldwide have embraced ICP-MS instrumentation because it gave low limits of detection for elemental analysis that were previously unavailable. Since then, Agilent has been working to improve the technology and ease of use to give customers more reliable results (Figure 1). The introduction of cool plasma, extended dynamic range detectors, collision/reaction cell with helium (He), and the High Matrix Introduction (HMI and UHMI) accessories have made ICP-MS easier to use and improved data quality. This has resulted in an increase in the presence of ICP-MS instruments in laboratories worldwide.

Today, Agilent ICP-MS systems combine the simplicity of a single collision cell mode for polyatomic interference removal with the superior matrix tolerance of its unique HMI system.

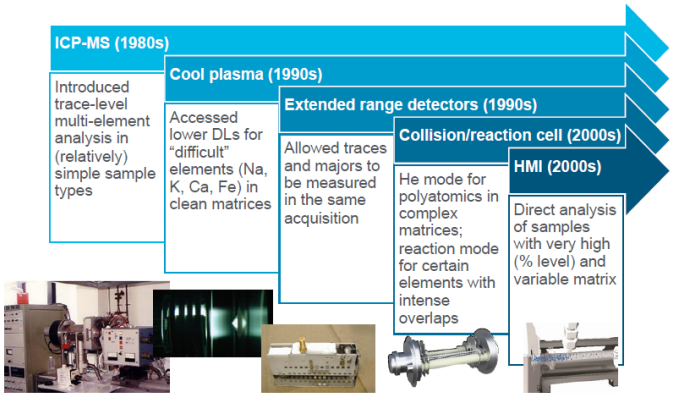

Figure 1. Highlights of continuous technical improvement in ICP-MS performance.

The fourth-generation Octopole Reaction System (ORS^4) cell technology provides higher sensitivity and more effective interference removal than ever before in complex, high matrix environmental samples. Helium mode on the ORS^4 is so effective that the need for interference equations can be virtually eliminated. These two factors redefine ease of use in ICP-MS, removing two of the most common causes of errors in multi-element analysis of complex samples.

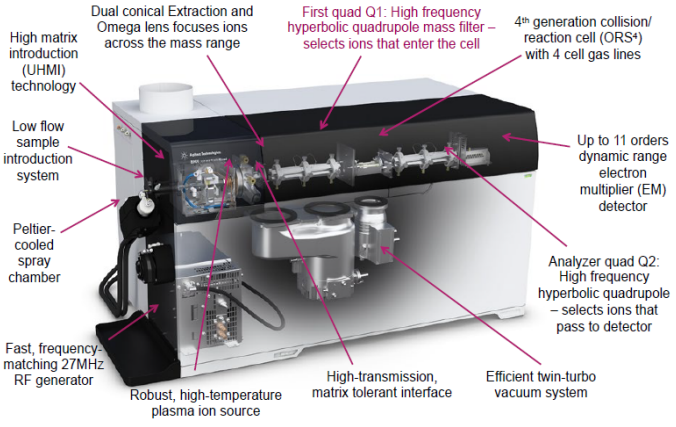

Figure 2. Controlling what enters the reaction/collision cell.

Defining the Future of ICP-MS

Agilent continues to innovate ICP-MS technology to address not only today's needs, but also to meet future demands for sensitivity, selectivity, and elimination of interferences. Agilent's customer-centric research and development has led to the introduction of the first triple-quadrupole ICP-MS system on the market. This instrument has two fully functional and interchangeable quadrupoles before and after the reaction/collision cell, as shown in Figure 2.

When introduced in 2012, the Agilent 8800 ICP-QQQ system included all the capabilities of the best-selling single-quad ICP-MS systems. It can analyze samples containing up to 3% total dissolved solids, has a dynamic range of up to 10 orders of magnitude, and has the same He collision mode capabilities.

In addition, a fully functional quadrupole was placed before the reaction cell to help control what enters the cell and help analysts better predict what will happen in the cell. Another benefit that this instrument provides is the improvement of Abundance Sensitivity (the ability of a quadrupole to resolve the contribution from adja cent masses). Since the abundance sensitivity will be the product of quadrupoles in series, having two fully functional and interchangeable quadrupoles with 10^{-7} resolving power in series means an abundance sensitivity >10^{-10}. With these unique capabilities, the 8800 ICP-MS system was quickly embraced by premier laboratories worldwide.

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In 2016, the second-generation ICP-QQQ instrument (the Agilent 8900 ICP-QQQ) was introduced to the market with new and improved capabilities. With higher sensitivity and lower background, the 8900 ICP-QQQ instrument can now analyze up to 25% solids with the UHMI Accessory. The new, faster detector not only has an extended linear dynamic range (up to 11 LDR), but also provided unprecedented capability, which can be applied to never imagined applications in emerging nanoparticle technology research. The new generation ORS with optional Axial Acceleration adds even more control of reaction in the cell.

The optional inert Ar flow system now achieves detection limits for elements like sulfur and silicon in the low ppt concentration range.

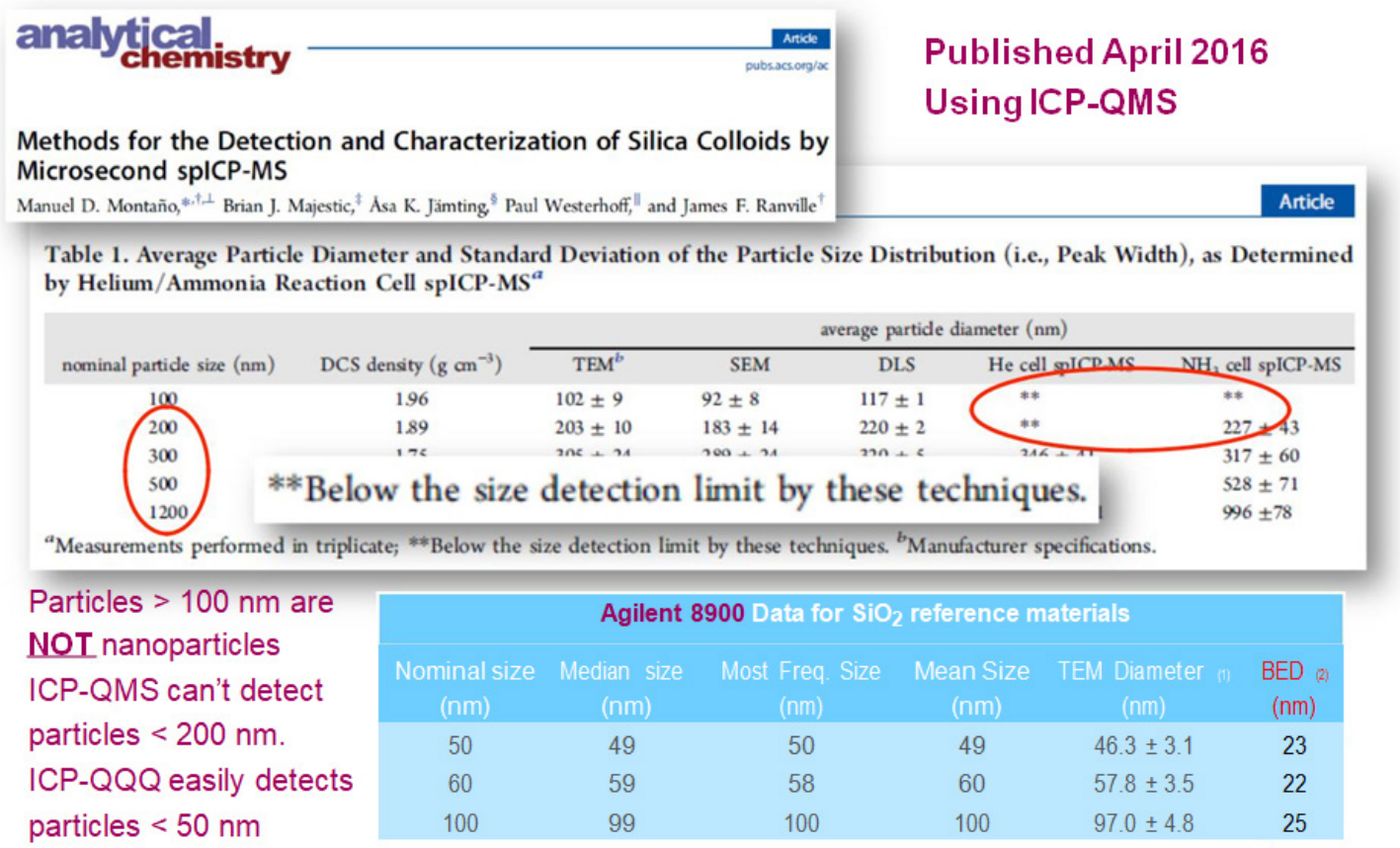

Figure 3. SiO_2 NP comparison ICP-QMS versus 8900.

Combined with the power to perform true MS/MS capabilities, these new capabilities allow laboratories to analyze some elements at lower levels than ever before. For instance, analysts can now determine silicon nanoparticle diameters at much lower levels with much greater accuracy than with other techniques in the market. By comparison, the single-quad instrument with bandpass could not trully determine anything below 200 nm, which excludes nanoparticles by definition (Figure 3).

The added capabilities provide analytical laboratories with tools not available before now. What specific capabilities of the Agilent 8900 ICP-QQQ instrument are driving the future of ICP-MS technology?

Capability One: MS/MS On-Mass Mode. With the MS/MS On-Mass Mode, the instrument removes an interference by moving the interference away from the element of interest. The first quadrupole is set to target mass, allowing only the analyte and on-mass interferences to enter the cell. The second quadrupole is also set to the target mass, measuring the analyte after the interferences have been removed by reaction in the cell. As an example, an analysis of mercury in the presence of tungsten was examined, where even small amounts of tungsten can create a false reading for mercury. With the Agilent 8900 instrument, the first quadrupole is set to 202 allowing only the Hg^{202} and the WO^{202} to enter the cell where WO^{202} is reacted away.

The second quadrupole, set at 202, eliminates any other ions that may have formed in the reaction cell. With the 8900 ICP-QQQ instrument, only the mercury reaches the detector. As a comparison, a single quadrupole or a bandpass ICP-MS would allow W^{186} to enter the cell creating new WO^{202}. With a single quad or a bandpass, the analyst does not have the confidence that only Hg is detemined.

Capability Two: MS/MS Mass-Shift Mode. The second capability is MS/MS Mass-Shift Mode, which is used when the analyte is reactive and the interferences are not reactive. With MS/MS Mass-Shift Mode the element of interest is moved

away from the interference. The first quadrupole is set to the target mass, controlling the ions that enter the cell and react. The second quadrupole is set to the mass where the easured reaction will land. Figure 4 shows a side-by-side example in which titanium is separated from all the potential overlaps with the product ion using this capability on the ICP-QQQ instrument. In comparison, a single-quadrupole or a bandpass ICP-MS instrument would allow all other masses to reach the cell, thus hampering analysis confidence that titanium is the only ion reaching the detector.

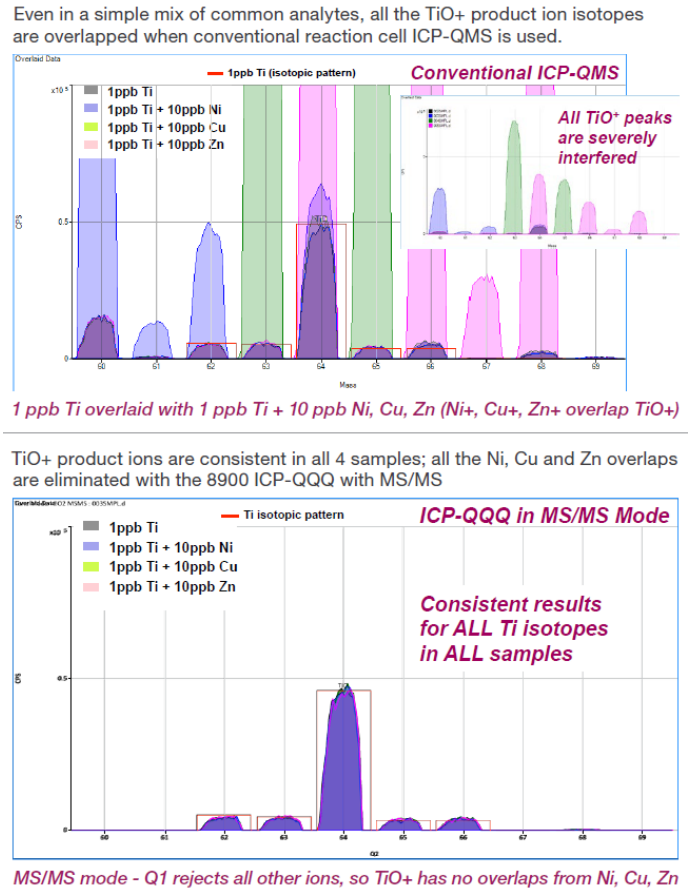

Figure 4. Comparison of single quad vs MS/MS operation TiO_+ product ions with O_2 cell gas.

Capability Three: Precursor Ion Scanning. Precursor Ion Scan is the third capability that is defining the future of ICP-MS equipment. Precursor Ion Scan is an excellent tool to find the source of a signal. With Precursor Ion Scan, the second quadrupole is set to the mass of interest while the first quadrupole scans the entire mass range. This new tool for troubleshooting can easily identify the source of unknown peaks. A very simple example is the use of the Precursor Ion Scan to identify the source of a peak interfering at 105 (even in DI water). Setting the second quadrupole to 105 and scanning the first quadrupole, mass by mass, revealed that only mass 89 produced the peak at 105. The operator realizes that the internal standard Y^{89} is the source of signal at 105 (YO^{105}). The operator may be able to deliberate to solve this type of problem, but the power of this capability is phenomenal for more complex and difficult problems, which would not be easily resolved otherwise.

Capability Four: Product Ion Scan. The fourth capability is the Product Ion Scan, which is a useful tool for a novice user to become a method development expert in complex matrices. A reaction gas, such as ammonia, is added to the reaction cell. The second quadrupole scans the entire range to find the strongest product ions signals. This unique capability enables the user to find the mass where the element of interest roduces a strong signal and nothing else interferes with the analyte. This capability greatly streamlines the workflow and simplifies method development.

Considering Isotopes

Isotope selection is second nature for experienced ICP-MS analysis. Experience has taught which isotopes have good abundance and which isotopes to use for each matrix to avoid overlaps. However, there are times when more than one isotope may be needed. For example, confirming isotopes are often used to validate data. Unfortunately, there are often no good confirming isotopes available and there may not be any other isotopes at all (like in monoisotopic elements), so new ways to increase confidence in results are adopted.

One novel application of MS/MS instrumentation has been the use of metal oxides to confirm results, even for monoisotopic elements. A metal when exposed to naturally abundant oxygen should form an oxide that mirrors oxygen itself. For example, yttrium when exposed to oxygen should form $Y^{89}O^{16}$ $Y^{89}O^{17}$ and $Y^{89}O^{18}$ that mirrors O^{16}, $O^{17,}$ and O^{18} (Figure 5).

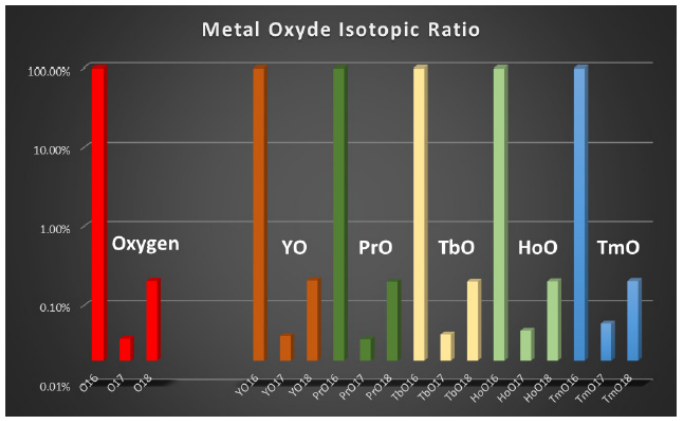

Figure 5. Confirming accuracy by O_2 natural abundance.

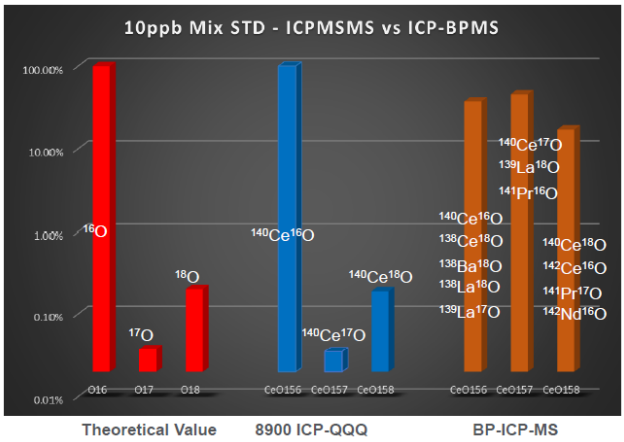

Figure 6. Effective MSMS vs bandpass.

The Agilent 8900 with true MS/ MS capability is the only instrument on the market capable of reliably achieving these ratios. Since the O^{17} is only 0.038% and O^{18} is 0.205%, it is imperative that the instrument controls what enters the cell within 1AMU while maintaining high sensitivity. Having high sensitivity or a bandpass will not achieve the same results.

How can you determine if an instrument has this capability? A quick test to confirm if an instrument can yield these types of results is to analyze 10 ppb cerium and plot the oxides formed. Only an instrument with fully functional and exchangeable quadrupoles before and after the cell can achieve $Ce^{140}O^{16}$ $Ce^{140}O^{17}$ and $Ce^{140}O^{18}$ ratios that mirror oxygen because the instrument is only allowing Ce^{140} to enter the cell and nothing else. A single-quadrupole or a bandpass system will allow other Ce isotopes to enter and react in the cell. This means that the signal at *m/z* 156 will be a combination of $Ce^{138}O^{18}$ and $Ce^{140}O^{16}$ and the signal at 158 will be a combination of $Ce^{142}O^{16}$ and $Ce^{140}O^{18}$. This quick test will show that the instrument has the capability of fully controlling what enters and reacts in the cell. Figure 6 shows how even with the addition of other rare earth elements and barium, the Agilent 8900 ICP-QQQ instrument still excels at this confirmation testing.

Conclusion

While the ICP-MS technique has been embraced by analysts for years, the increased sensitivity as well as the four new capabilities of the Agilent 8900 ICP-QQQ instrument are defining the future of ICP-MS technology. This system simplifies method development and streamlines workflows, while meeting the needs for increased sensitivity and accuracy, especially in the presence of complex sample matrices.

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