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A comprehensive guide to method development using triple quadrupole ICP-MS

Introduction

Inductively Coupled Plasma Mass Spectrometry (ICP-MS) is recognized as a key technique for the analysis of trace elements in a wide variety of sample types. This is due to its outstanding speed, detection sensitivity and ability to achieve detection limits generally in the low ng·L¹ concentration range for most of the elements in the Periodic Table. For a number of elements, in particular metals with low ionization potential and low natural backgrounds, detection limits in the pg·L¹ range can be achieved, even under normal laboratory conditions. Using a suitable configuration of the sample introduction system, the introduction of even the most challenging sample types, such as soil digests or undiluted sea water (total amount of dissolved solids approximately 3.5%), is possible. ICP-MS is therefore considered the major technique for sensitive and high throughput analysis. However, biased or false positive results are still of concern for operators, lab managers and researchers, and in many cases, the root cause is unresolved spectral interferences. This is especially true for monoisotopic or quasi-monoisotopic elements, such as arsenic, which is a key analyte in many regulated methods governing the safety of, for example, drinking water, foodstuffs or pharmaceutical products.

After continuous improvement in interference removal through the use of single quadrupole ICP-MS instrumentation equipped with a collision/reaction cell (such as the Thermo Scientific™ iCAP™ RQ ICP-MS), recent years have seen accelerated development of ICP-MS using triple quadrupole technology (such as the Thermo Scientific™ iCAP™ TQ ICP-MS). These systems allow for consistent interference removal regardless of the sample matrix. Developments in hardware and software focusing on ease of use in routine trace elemental determinations have allowed for triple quadrupole ICP-MS to be adopted by increasing numbers of laboratories. Here, they are taking over analysis from established techniques, such as Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) and single quadrupole ICP-MS.

This compendium will show you the options and best solutions to analyze a full suite of elements (non-naturally occurring elements excluded) in any sample matrix, using triple quadrupole ICP-MS. For each element, a brief description of the isotopes available for analysis as well as common and less common interferences will be included. Finally, a table will highlight how each of the elements can be successfully analyzed.

Example for the table format used throughout this document

Element	Barium	
Available isotopes	¹³⁰ Ba (0.11%), ¹³² Ba (0.10%), ¹³ ¹³⁶ Ba (7.85%), ¹³⁷ Ba (11.2	
Ionization Potential	5.21 eV (10.00 eV)	
Q1 resolution 3	Intelligent Mass Selection (iMS)	
Dreferred analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED 4	TQ-O ₂ (138Ba16O)

The information shown in this compendium plus a wide variety of other, additional possible reactions for all elements in the periodic table is stored in the Reaction Finder method development assistant included in the Thermo Scientitific™ Qtegra™ Intelligent Scientific Data Solution Software and is accessible anytime for consistent method development even for inexperienced users. This includes optimized settings for all relevant parameters, such as reactive gases, possible product ions (if any) and Q1 resolution.

- 1 All available isotopes with isocratic abundance are shown. The preferred isotope is shown in bold.
- 2 The ionization potential indicates potential ion yield. Numbers in parentheses indicate that double charged interferences can be formed by this element.
- 3 Resolution setting when triple quadrupole modes are used for analysis
- 4 Best and alternative choice for the analysis of a given element—potential changes in product ions are mentioned in parentheses.

General conditions—how plasma conditions and sample matrix influence the analysis

One of the reasons for the wide applicability of ICP-MS as a technique for the analysis of trace elements is its high sensitivity combined with unique robustness, enabling the analysis of a variety of sample matrices without (or at least with reduced) matrix effects, in comparison to techniques such as organic mass spectrometry. Matrix effects caused by a change of the sample matrix still occur but can be reduced by choosing the right configuration of the sample introduction system and compensated for by using suitable internal standards.

The matrix tolerance of ICP-MS is achieved as a result of the high plasma temperature enabling full decomposition of the sample matrix to (mainly) singly charged atomic ions, in the general form M*. Every element with an ionization potential lower than the first ionization potential of argon (15.76 eV) should form ions in an argon generated plasma. However, the lower the ionization potential of an element is, the higher is the degree of ionization, and therefore the sensitivity. Some elements show 2nd ionization potentials well below the ionization potential of argon, so that a significant formation of doubly charged ions is observed, which in turn can lead to interferences on other elements. Tuning the plasma to a high temperature allows rapid and effective decomposition of the sample matrix leading to robust and reliable analysis of complex sample matrices, such as food digests, drinking waters or soil digests.

The actual temperature of the plasma is impossible to measure, but generally ranges between 6,000 to 10,000 K depending on the tuned conditions. For the iCAP RQ ICP-MS and iCAP TQ ICP-MS systems, the typical plasma temperature can be estimated to be between 7,500 and 8,000 K (using the standard sample introduction system). Factors influencing the plasma temperature include the RF power, the plasma gas flows, the size of the injector tube etc. Also, the sample flow and the sample matrix play an important role, as a too high sample flow or a complex matrix may consume a significant amount of energy from the plasma and hence reduce the available energy for ionization of critical elements, especially those with elevated ionization potential (\geq 8 eV). The correlation between the degree of ionization and the ionization potential for a given plasma temperature can be calculated using the so-called Saha-Langmuir equation. Assuming a plasma temperature of 8,000 K, the following ionization efficiencies are typically observed (Table 1).

Table 1: Dependency of the ionization efficiency from the ionization potential at a typical plasma temperature of 8,000 K

Ionization potential	Degree of ionization	Examples
Below 6 eV	100%	Alkaline and alkaline earth elements, lower rare earth elements
Between 6-8 eV	Close to 100%	Transition metals, noble metals, higher rare earth elements
Between 8–10 eV	Decreasing to about 50%	Some metals such as zinc, palladium, cadmium, antimony, osmium, iridium, platinum, gold. Semi-metals and non-metals (e.g., beryllium, boron, silicon, arsenic, selenium, tellurium).
Higher than 10 eV	Below 50 % (10% @ 12 eV)	Mercury as the only metal. Non-metals like carbon, nitrogen, oxygen, sulfur and phosphorous, but also halogens such as chlorine and bromine

The conditions of the plasma are often characterized by indicators such as the formation rate of oxides (using for example the 140 Ce16 O+/140 Ce+ ratio) and doubly charged ions (using the M**/M* ratio an element with a low 2nd ionization potential, such as Ba or Ce). However, these two factors are closely dependent on each other and it is not possible to tune an inductively coupled plasma to reduce both of them at the same time. An increase in the plasma temperature may help to reduce the amount of oxides formed, but it will increase the extent of formation of doubly charged ions and vice versa. Although a higher plasma temperature would allow for potentially higher sensitivity for elements with elevated ionization potential, a higher formation of doubly charged ions, leading to interferences, would be observed as well. Tuning (manual or automated) of an inductively coupled plasma for mass spectrometry therefore takes both into account. Generally, a well-tuned ICP-MS system achieves a formation of oxides of typically less than 2% (1.5-2.0%), with doubly charged ions below 3.0% at the same time (typically between 2.5 and 3.0%). As many elements form oxides or doubly charged ions, a wide variety of interferences need to be overcome because of their formation in the plasma.

Spectral interferences and how to overcome them

Spectral interferences commonly observed in ICP-MS include polyatomic ions, doubly charged ions or isobaric interferences. In some cases, with very intense signals observed on a mass adjacent to the analyte mass, an overlap of the neighboring signal might be observed as well.

- Polyatomic interferences are formed through recombination of previously ionized atoms as the ion beam traverses the interface region (e.g., between sample and skimmer cone). Expansion into the vacuum (from atmospheric pressure to about 2 mbar and subsequently to 10⁻⁷ mbar in the mass analyzer) leads to cooling of the ion beam, and hence recombination reactions can occur. Polyatomic interferences may be formed from all elements present in the sample, but the most severe polyatomics are created from argon ions in conjunction with O⁺, and H⁺ derived from the aqueous sample media, or if present, N⁺, Cl⁺, S⁺ derived from the acid matrix.
- Doubly charged interferences are formed through secondary ionization of elements with particularly low ionization potential. As all mass spectrometers detect ions on the basis of their mass to charge ratio (rather than mass alone), they will impact analytes at half the mass of the interfering element. These interferences are however easy to recognize in a mass spectrum.

Whereas polyatomic and doubly charged ions are formed in the plasma and their signal level can, to some extent, be controlled by the plasma conditions, isobaric interferences are caused by other elements present in the sample sharing isotopes with identical mass number and cannot be influenced by the instrument at all. However, in most cases they can be corrected for using correction equations, provided that another isotope of the interfering element is available and is itself free from interferences.

A common approach to interference removal is kinetic energy discrimination (KED, Figure 1): Interference removal is achieved using helium in the collision reaction cell. All ions traveling through the cell sustain collisions with helium, although through its inert nature, no chemical reactions are induced. A positive bias potential is applied between the CRC and the analyzing quadrupole, so that only ions with sufficient kinetic energy remaining will exit the cell.

Polyatomic interferences will be efficiently suppressed as they have a higher collisional cross section and lose more kinetic energy along the way. KED is even more effective when used in combination with a low mass cut off to eliminate ions of lower mass in the CRC, in order to reduce the formation of additional interferences in the cell. KED is an effective tool for the removal of polyatomic interferences, however, other types of interferences, such as isobaric overlaps or doubly charged ions are not eliminated.

Triple quadrupole systems can also leverage KED in the same way as a single quadrupole ICP-MS. In KED mode on a triple quadrupole system, the first mass filtering quadrupole is operated as an ion guide only.

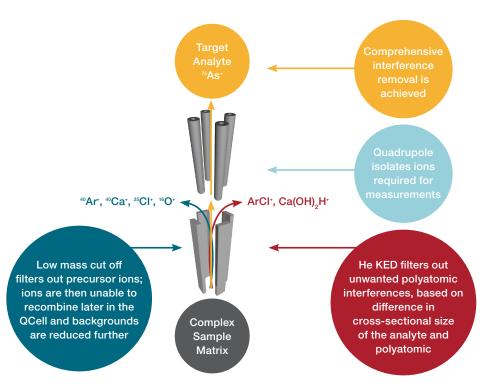


Figure 1: Interference Removal using Kinetic Energy Discrimination on the iCAP RQ ICP-MS.

Triple quadrupole ICP-MS systems such as the iCAP TQ ICP-MS achieve a new level of data quality and confidence in the result, and hence allow a significant improvement for key elements.

Interference removal based on triple quadrupole technology (also occasionally referred to as MS/MS) includes a mass filtration step before the collision/ reaction cell, removing all ions of lower and higher mass than the analyte and its interferences with identical mass to charge ratio. This initial mass filtration allows reactive gases to be used for interference removal, which can induce highly selective ion-molecule reactions between either the analyte or the interfering ions with the gas. This will lead to a change of the ions observed, and hence a second mass filtration step in the analyzing quadrupole will allow the interference to be fully eliminated. The process of interference removal on the iCAP TQ ICP-MS is illustrated in Figure 2:

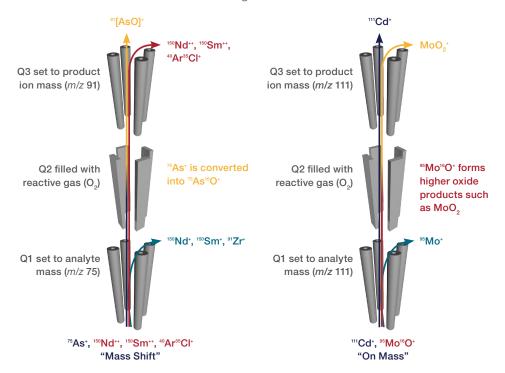


Figure 2: Possible reaction pathways in triple quadrupole ICP-MS.

The decision on whether a mass shift of the analyte (a so-called mass shift reaction) occurs or whether the interfering ions will react (a so-called on mass reaction) highly depends on the reactive gas used. Different gases exhibit different reactivities to certain ionic species, in many cases forming simple product ions, such as oxides (addition of an atom of oxygen), but also in other cases, complex product ions. The latter is in particular observed with ammonia, allowing very selective ion/molecule reactions with a variety of elements, but also effectively reducing charged ionic species, such as some polyatomic species. The following gases are typically used in conjunction with triple quadrupole ICP-MS:

- Oxygen (O₂): O₂ induces a variety of effective chemical reactions with different elements. For the most cases, an oxidation reaction will occur, leading to a mass shift of the analyte (e.g., ⁷⁵As will be converted into ⁷⁵As¹⁶O). This allows for effective suppression of polyatomic as well as doubly charged ions. Differences in the reactivity towards oxygen can be used in order to remove isobaric overlaps, such as the removal of ⁸⁷Rb from ⁸⁷Sr.
- Ammonia: Ammonia (NH₃) can react in different ways. Whereas with some elements, such as titanium, it forms a wide variety of reaction products (for example [TiNH(NH₃)x], it can also effectively eliminate polyatomic (especially chlorine based) polyatomics. The removal of isobaric overlaps is as well possible, for example, the elimination of ²⁰⁴Hg from ²⁰⁴Pb.
- **Hydrogen:** Although used for reduction of the ⁴⁰Ar₂⁺ interference (affecting the detection of ⁸⁰Se), the use of hydrogen is not leading to a significant performance improvement on triple quadrupole ICP-MS systems. Some elements, such as chlorine or phosphorous, may react in a mass shift reaction (to form CIH₂⁺ or PH₂ / PH₄⁺), the yield is often low in comparison to a mass shift reaction with oxygen. Nevertheless, for some applications, the use of H₂ can be beneficial.

In some cases, special analysis conditions can also help to improve the overall performance of the ICP-MS analysis.

Out of the common toolbox for removing spectral interferences, there are a number of techniques that can allow significant improvements, but may only be applicable for a very limited set of sample matrices:

• Cold (or cool) plasma uses a reduction of the RF power from about 1500 W to typically less than 700 W in order to reduce the plasma temperature and hence the ionization of argon. Cold plasma conditions will typically favor the ionization of elements with low ionization potential, especially alkaline and alkaline earth elements such as Na, K, or Ca. In conjunction with the reduced observation of argon based polyatomic species, a significant reduction of backgrounds and detection limits is possible. However, cold plasma conditions can only be applied for pure samples without any matrix load, for example in the impurity screening of process chemicals in the semiconductor industry.

• Adjustable quadrupole resolution settings can help to reduce the intense signals obtained from the measurement of major components in a sample. The resolution of the analyzing quadrupole can typically be reduced from the standard setting of about 0.7 amu to about 0.3 amu almost instantly during the analysis. In addition, an increase of the resolution setting allows the negative effect of peak tailing of highly abundant signals adjacent to an analyte, more commonly known as abundance sensitivity of the mass spectrometric system, to be reduced.



Periodic Table of elements































Lä

Sc





Zr

Hf



Nb

Ta



using triple quadrupole ICP-MS.



Mo

W¹

Tunasten

















Au



























































































Ne

Kr³⁶

Krypton

Xe

Xe







Ge



As

Sb



O

Së

Të



F°

Br



T⁴³

Re

Click on any of the elements in red to jump to the specific page to read more information on method development



Rü

Os Os



Rh

lr"

Iridium



Pď







Hg

Z'n





Gå









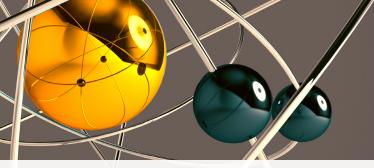












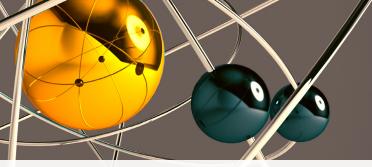
Lithium, Beryllium, Boron

Elements with low mass rarely benefit from the use of a reactive gas, since interferences are rare and interaction with heavier gas molecules (such as O₂ or NH_a) would lead to a significant reduction of sensitivity. Generally, these elements can be analyzed using either standard (no cell gas mode) or KED mode. Although there is a loss of sensitivity in KED mode for these low mass ions, detection limits in the low ng·L¹ range are still achievable as backgrounds are reduced as well. This enables a reduction of the overall run time for multi-element analysis as there is no need to include an additional switch to standard mode. Whereas beryllium is monoisotopic, both lithium and boron have two isotopes, of which the heavier isotope in both cases has a significantly higher abundance. The minor isotope of lithium is available as an enriched stable isotope standard and is allowed for use as an internal standard for low mass elements within a number of regulatory guidelines (such as EPA method 200.8). For boron, interferences can arise from the presence of organic solvents (from peak tailing of the neighboring, very intense ¹²C signal) or in the presence of high levels of Mg, (formation of ²⁴Mg⁺⁺ at mass 12 with tailing into ¹¹B). The use of a second mass filtration step using Q1 can improve the resolution of the adjacent signal, even without the use of the CRC or any collision/reaction gas.

Element	Lithium		
Available isotopes	°Li (7.50%), 7 Li (92.50%)		
Ionization Potential	5.39 eV		
Q1 resolution	1 amu		
Duestoure de control de control	Reaction Finder Default	Alternatives	
Preferred analysis modes	SQ-KED	SQ-N/A	
Element	Beryllium		
Available isotopes	°Be (100%)		
Ionization Potential	9.32 eV		
Q1 resolution	1 amu		
Duefe weed a selection and a	Reaction Finder Default	Alternatives	
Preferred analysis modes	SQ-KED	SQ-N/A	
Element	Boron		
Available isotopes	¹⁰ B (19.90%), ¹¹	¹⁰ B (19.90%), ¹¹ B (80.10%)	
Ionization Potential	8.30 eV		
Q1 resolution	1 amu		
Duefermed analysis and de-	Reaction Finder Default	Alternatives	
Preferred analysis modes	SQ-KED	SQ-N/A, TQ-N/A	







Sodium

Sodium is monoisotopic at m/z 23. Although no significant interferences are expected, sodium is usually analyzed using KED mode (in e.g., environmental or food samples) for attenuation of the high signals caused by its ubiquitous nature. This can also be combined with increased resolution of the analyzing quadrupole to further reduce the signal intensity and increase the dynamic range even more. Where trace or ultra-trace analysis is required (for example in the semiconductor industry) the use of cold plasma conditions can lead to a significant improvement of detection sensitivity and limits of detection.

Element	Sodium	
Available isotopes	²³ Na (100%)	
Ionization Potential	5.14 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Preferred analysis modes	Reaction Finder Default	Alternatives
	SQ-KED	SQ-N/A, TQ-O ₂ (²³ Na)

Magnesium

Magnesium has three isotopes, of which $^{24}\mathrm{Mg}$ is the default choice for analysis. Although polyatomic interferences are unlikely to occur (with the exception of $^{12}\mathrm{C_2}^+$ formed when analyzing organic solvents), there may be a potential bias caused by $^{48}\mathrm{Ca}^{++}$ in (e.g., environmental samples). Magnesium does show a reduced reactivity to $\mathrm{O_2}$ compared to higher alkaline earth elements, but the use of $\mathrm{O_2}$ followed by on mass analysis allows the aforementioned interferences to be comprehensively removed.

Element	Magnesium	
Available isotopes	²⁴ Mg (78.99%), ²⁵ Mg (10.00%), ²⁶ Mg (11.01%)	
Ionization Potential	7.65 eV (15.03 eV)	
Q1 resolution	1 amu	
Droformed analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-O ₂ (²⁴ Mg)







Aluminum

Aluminum is monoisotopic with its only isotope ²⁷Al. This element may be interfered in carbon containing solutions (arising from ¹²C¹⁴N'H'), but generally it is not affected by significant overlaps. However, aluminum can show sample matrix related errors, such as high signal fluctuation in the case of low sample acidity, as a result of the formation of Al colloids under these conditions. Often times, the addition of a small amount of acid can help to overcome this potential issue.

Element	Aluminum	
Available isotopes	²⁷ AI (100%)	
Ionization Potential	5.99 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Preferred analysis modes	Reaction Finder Default	Alternatives
	SQ-KED	SQ-N/A, TQ-O ₂ (²⁷ AI)

Silicon

Silicon is one of the most difficult elements for ICP-MS analysis, mainly because of the ubiquitous nature of this element and the need to carefully control blank levels. The major potential interferent is nitrogen from ambient air (forming an $^{14}\mathrm{N_2^+}$ interference on the major isotope of silicon, $^{28}\mathrm{Si}$). Although other isotopes of silicon are less interfered ($^{29}\mathrm{Si}$ and $^{30}\mathrm{Si}$), their low natural abundance limits the attainable detection sensitivity. The choice of the most appropriate mode for analysis strongly depends on the sample matrix. Whereas for aqueous samples, the use of TQ-H $_2$ (on mass reaction) allows to effectively suppress the $^{14}\mathrm{N}_2^+$ interferences, for organic solvents, the choice of TQ-O $_2$ mode is superior. Silicon can react with O $_2$ to from $^{28}\mathrm{Si}^{16}\mathrm{O}$, however, $^{12}\mathrm{C}^{16}\mathrm{O}$ as a potential interferent would react likewise to form $^{12}\mathrm{C}^{16}\mathrm{O}_2$ with an equal m/z ratio. Therefore, detection of $^{28}\mathrm{Si}^{16}\mathrm{O}_2^+$ is often providing superior results. Therefore, the best way for the analysis of silicon is the use of H $_2$, leading to charge neutralization of the polyatomic interferences, or, the use of the minor $^{29}\mathrm{Si}$ isotope in conjunction with O $_2$.

Element	Silicon	
Available isotopes	²⁸ Si (92.23%), ²⁹ Si (4.67%), ³⁰ Si (3.10%)	
Ionization Potential	8.15 eV	
Q1 resolution	1 amu	
	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-H ₂ (²⁸ Si), TQ-O ₂ (²⁸ Si ¹⁶ O ₂)







Phosphorous

Phosphorous is an important element due to its role in nutrition. It is also a highly relevant element in life science applications, as it can act as a proxy for DNA or DNA fragments, or be used for the detection and quantification of post-translational modifications of proteins through phosphorylation. However, due to its high ionization potential and significant polyatomic interferences (principally $^{14}\text{N}^{16}\text{O'H'}$), the analysis of phosphorous is often limited by reduced detection sensitivity and elevated detection limits. Due to its monoisotopic nature, there are no less interfered alternative isotopes available. However, phosphorous reacts efficiently with O_2 and hence the majority of polyatomic interferences can be separated on a triple quadrupole ICP-MS system with dramatically improved sensitivity.

Element	Phosphorous	
Available isotopes	³¹ P (100%)	
Ionization Potential	10.49 eV	
Q1 resolution	1 amu	
Preferred analysis modes	Reaction Finder Default	Alternatives
	TQ-O ₂ (³¹ P ¹⁶ O)	SQ-KED, TQ-H ₂ (³¹ P ¹ H ₂)

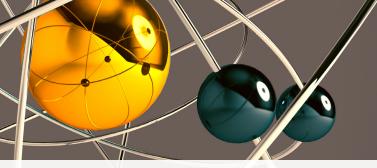
Sulfur

Sulfur is one of the most difficult elements to be analyzed using ICP-MS. Because of its high ionization potential, the ion yield is generally low, and in aqueous media, there are highly abundant interferences, such as $^{16}\mathrm{O_2^*}$. Although the interferences on $^{34}\mathrm{S}$ are less pronounced ($^{16}\mathrm{O}^{18}\mathrm{O}$), the sensitivity is also reduced considerably because of the lower abundance of the isotope. The use of $\mathrm{O_2}$ and a mass shift reaction forming $^{32}\mathrm{S}^{16}\mathrm{O}$ can substantially improve the detection limits (typically, sub ppb levels are achieved), but mass filtration is essential to avoid interferences on the product ion mass through $^{48}\mathrm{Ti}$ or $^{48}\mathrm{Ca}$.

Element	Sulfur	
Available isotopes	³² S (95.02%), ³³ S (0.75%), ³⁴ S (4.21%), ³⁶ S (0.02%)	
Ionization Potential	10.36 eV	
Q1 resolution	1 amu	
Dueste was diene land in in mende	Reaction Finder Default	Alternatives
Preferred analysis modes	TQ-O ₂ (32S16O)	SQ-KED (³⁴ S)







Chlorine

Chlorine is an untypical element to be analyzed using ICP-MS. This is mainly due to its high ionization potential leading to low ion yield from the plasma and hence low sensitivity. In addition, hydrochloric acid is often an integral part of sample preparation. Nevertheless, chlorine can be analyzed using ICP-MS, for example to confirm its absence in process chemicals in the semiconductor industry. The principal interferences on Cl are '¹⁷O₂'H⁺ on ³⁵Cl and ³⁶Ar'H⁺ on ³⁷Cl, with the latter interference being proportionately higher. The less interfered ³⁵Cl isotope is also the more abundant, so is preferred for analysis. The use of triple quadrupole systems is beneficial for Cl analysis because of a positive effect on sensitivity through ion focusing and acceleration in the CRC. Chlorine can form product ions with both oxygen (e.g., ³⁵Cl'¹⁶O⁺) and hydrogen (e.g., ³⁵Cl'H₂⁺), the latter being less effectively formed as two subsequent reaction steps are required for its formation.

Element	Chlorine	
Available isotopes	³⁵ Cl (75.77%), ³⁷ Cl (24.23%)	
Ionization Potential	12.97 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Preferred analysis modes	Reaction Finder Default	Alternatives
	TQ-O ₂ (35Cl ¹⁶ O)	TQ-H ₂ (35Cl1H ₂)

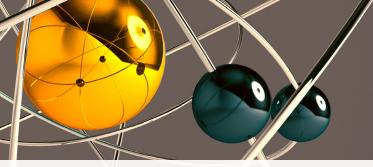
Potassium

Potassium has its main isotope at m/z 39. Due to the adjacent and highly intense signal caused by the main isotope of argon (40Ar), there may be a contribution at low K levels from peak tailing. However, there is also direct, onmass contribution from 38Ar'H*. If the analysis of potassium at ultra-trace levels is required, for example, in the semiconductor industry, cold plasma can be used to reduce the formation of both 40Ar* and 38Ar'H* ions and hence allow more sensitive detection of K.

Element	Potassium	
Available isotopes	³⁹ K (93.26%), 40K (0.01%), 41K (6.83%)	
Ionization Potential	4.34 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Preferred analysis modes	Reaction Finder Default	Alternatives
	SQ-KED	Cold Plasma







Calcium

Calcium has several different stable isotopes with masses between 40 and 48. The most abundant isotope ⁴⁰Ca is interfered through ⁴⁰Ar and hence not accessible when using hot plasma conditions. For typical applications, although limited in abundance, the ⁴⁴Ca isotope is used for analysis. The main polyatomic interferences on this isotope are caused through ¹²C¹⁶O₂⁺, ²⁸Si¹⁶O⁺. ²⁷Al¹⁶O¹H⁺ or ³²S¹²C⁺, but there are also potential doubly charged overlaps with ⁸⁸Sr⁺⁺ or ⁸⁹Y⁺⁺. As for potassium, cold plasma can be used to reduce the formation of ⁴⁰Ar⁺ ions and hence allow the analysis of the main isotope in cases where the sample matrix concentration is low.

Element	Calcium	
Available isotopes	⁴⁰ Ca (96.94%), ⁴² Ca (0.65%), ⁴³ Ca (0.14%), ⁴⁴Ca (2.09%), ⁴⁶ Ca (0.004%), ⁴⁸ Ca (0.19%)	
1st Ionization Potential	6.11 eV (11.87 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-O ₂ (44Ca ¹⁶ O), TQ-NH ₃ (40Ca)

Scandium

Scandium is very attractive as a potential internal standard for the transition metals, as it is normally not present in most samples. However, its moderate 2nd ionization potential may lead to the formation of ⁴⁶Sc⁺⁺ ions, affecting the detection of ²⁹Na. Scandium can be interfered in the presence of phosphorous (³¹P¹⁴N⁺) and silicon (²⁹Si¹⁶O⁺), which may lead to misinterpretation of system stability when it is applied as an internal standard. Another potential influence on scandium is zirconium, as its major isotope, ⁹⁰Zr, may form doubly charged interferences.

Element	Scandium	
Available isotopes	⁴⁵ Sc (100%)	
Ionization Potential	6.56 eV (12.8 eV)	
Q1 resolution	1 amu	
Preferred analysis modes	Reaction Finder Default	Alternatives
Freierred analysis modes	TQ-O ₂ (45Sc16O)	SQ-KED, TQ-NH ₃ (45Sc)







Titanium

Titanium has a remarkable isotope pattern with a total of five stable isotopes, surrounding the most abundant isotope, 48 Ti. Due to a potential isobaric overlap with 48 Ca, and polyatomic interferences caused by $^{31}P^{16}O^{1}$ H or $^{32}S^{16}O^{+}$ in the presence of higher amounts of phosphorous and sulfur, respectively, the preferred choice on a single quadrupole system is often 47 Ti or 49 Ti. However, Ti reacts well with O_2 and NH_3 . Whereas the use of oxygen alone would lead to the formation of CaO+, and hence would not remove the interference of Ca (unless a combination of gases is used), titanium forms a variety of different product ions with NH_3 , the most abundant of them typically being $Ti[NH(NH_3)_3]^+$ and $Ti[NH(NH_3)_4]^+$, with mass to charge ratios of 114 and 131, respectively. If calcium is present in the sample as well, the reaction with NH_3 is therefore the preferred choice as Ca reacts only slightly with NH_3 .

Element	Titanium	
Available isotopes	⁴⁶ Ti (8.00%), ⁴⁷ Ti (7.30%), ⁴⁸ Ti (73.80%), ⁴⁹ Ti (5.40%), ⁵⁰ Ti (5.50%)	
Ionization Potential	6.83 eV (13.58 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-O ₂ (⁴⁸ Ti ¹⁶ O), TQ-NH ₃ (¹¹⁴ [⁴⁸ TiNH(NH ₃) ₃])

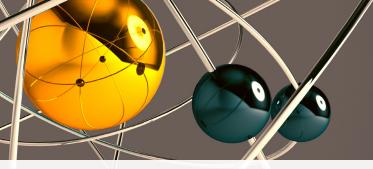
Vanadium

Vanadium has two stable isotopes, 50 V and 51 V, with 51 V being significantly more abundant. However, vanadium is strongly affected by interferences caused by chlorine through the formation of 35 Cl 16 O $^{+}$. This interference can be removed using KED or the use of a reactive gas (O $_2$ or NH $_3$). Whereas O $_2$ leads to a mass shift (51 V 16 O $^{+}$), the use of NH $_3$ improves the removal of the CIO interference, however, because V is not reactive towards NH $_3$, it can be measured on mass when this reaction gas is used. In presence of higher amounts of sulfur, the in most samples unlikely formed 34 S 16 O 1 H polyatomic interference can become a potential issue, fully removable through the use of triple quadrupole technology.

Element	Vanadium	
Available isotopes	⁵⁰ V (0.25%), ⁵¹ V (99.75%)	
Ionization Potential	6.75 eV (14.66 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
Drafarrad analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	TQ-O ₂ (⁵¹ V ¹⁶ O)	SQ-KED, TQ-NH ₃ (⁵¹ V)







Chromium

Similar to vanadium, chromium has one major isotope (52 Cr) and alternatives with lower abundance. The main isotope is mostly interfered by 40 Ar 12,13 C $^+$ in carbon rich sample matrices and, less heavily, by chlorine based interferences (e.g., 35 Cl 16 O 1 H or 37 Cl 16 O). Like vanadium, KED will efficiently remove the polyatomic overlaps, whereas O $_2$ and NH $_3$ also allow the detection sensitivity to be increased. When using O $_2$ as a reactive gas, a mass shift reaction is induced, whereas the element is measured on mass in conjunction with NH $_2$.

Element	Chromium	
Available isotopes	⁵⁰ Cr (4.35%), ⁵² Cr (83.79%)), ⁵³ Cr (9.50%), ⁵⁴ Cr (2.37%)
Ionization Potential	6.78 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Dreferred applyais mades	Reaction Finder Default	Alternatives
Preferred analysis modes	TQ-O ₂ (52Cr16O)	SQ-KED, TQ-NH ₃ (⁵² Cr)

Manganese

Although monoisotopic manganese is not affected by a major argon derived interference (40 Ar 14 N'H * is relatively low and 40 Ar 15 N $^+$ is almost negligible due to the low abundance of 16 N), there are interferences that need to be considered for certain sample types. In sample matrices containing higher amounts of potassium, the detection of manganese may be affected by the formation of 39 K' 16 O * . Samples containing elevated amounts of iron (such as whole blood) may lead to peak tailing of the neighboring isotopes 54 Fe and the more abundant 56 Fe. Whereas the polyatomic interferences are easy to remove, the removal of the peak tailing of iron will significantly benefit from the use of triple quadrupole technology with either O $_2$ or NH $_3$ (as manganese is not reactive to either of the gases), in combination with an increase of the resolution setting of the analyzing quadrupole mass filter.

Element	Manganese	
Available isotopes	⁵⁵ Mn (100%)	
Ionization Potential	7.43 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Drafarrad analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-O ₂ , TQ-NH ₃ (⁵⁵ Mn)







Iron

Iron has four stable isotopes, of which 56 Fe is the most abundant. However, when analyzing iron on a single quadrupole ICP-MS, often the less abundant isotope 57 Fe is the preferred choice, since 56 Fe is overlapped by an intense polyatomic interference, 40 Ar 16 O * . This interference can be reduced using KED, but signal to noise is often still favoring the alternative isotope. This overlap however can be efficiently reduced when applying a reactive gas such as O_2 or NH_3 . In this case, the argon based polyatomic interference will be neutralized in the cell, hence allowing the use of the most abundant isotope of iron.

Element	Iron	
Available isotopes	⁵⁴ Fe (5.80%), ⁵⁶ Fe (91 ⁵⁸ Fe (0.	
Ionization Potential	7.90 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Dreferred englysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-O ₂ , TQ-NH ₃ (⁵⁶ Fe)

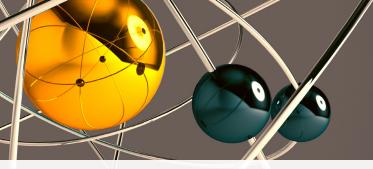
Cobalt

Cobalt is monoisotopic at mass 59. Due to its low ionization potential and the absence of any significant argon based polyatomic interferences, it can be analyzed with high detection sensitivity using kinetic energy discrimination. The presence of high amounts of nickel can lead to biased results through peak tailing (58Ni and 60Ni surrounding 59Co) and 58Ni'H+ formation, which can be resolved through the use of a reactive gas or the use of high resolution settings. Cobalt shows only a moderate reaction efficiency with oxygen, so an on mass measurement is the preferred choice when selecting triple quadrupole based modes.

Element	Cobalt	
Available isotopes	⁵⁹ Co (100%)	
Ionization Potential	7.88 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-O ₂ (⁵⁹ Co), TQ-NH ₃ (⁵⁹ Co)







Nickel

The main isotope of nickel is ⁵⁸Ni, however, the preferred isotope is in many cases ⁶⁰Ni to avoid an isobaric overlap with ⁵⁸Fe. Nickel is not seriously affected through polyatomic interferences in the majority of typical sample matrices and does not show extended reactivity towards the main reactive gases commonly used in triple quadrupole systems. The main choice for analysis is therefore the use of kinetic energy discrimination, but the use of ammonia may help to improve detection sensitivity in an on mass measurement.

Element	Nickel	
Available isotopes	⁵⁸ Ni (68.27%), ®Ni (26. 1 ⁶² Ni (3.59%), ⁶⁴ N	
Ionization Potential	7.64 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Drafarrad analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-NH ₃

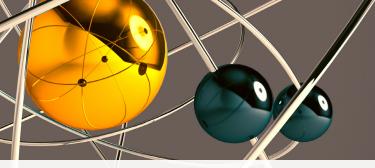
Copper

Copper has two isotopes, 63 Cu and 65 Cu. Whereas normally 63 Cu is the default choice, for the analysis of samples containing elevated amounts of sodium, the selection of 65 Cu may be beneficial, as 63 Cu can be affected by the formation of 40 Ar 23 Na * . Whereas the reactivity towards O_2 is limited, copper does form several cluster ions with ammonia, however, on mass measurement is also possible.

Element	Copper	
Available isotopes	⁶³ Cu (69.17%), ⁶⁵ C u (30.83%)	
Ionization Potential	7.73 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Dreferred englysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-NH ₃ (95[63CuNH(NH ₃)])







Zinc

Zinc has a total of five stable isotopes, with the default selection often being $^{\rm e6}{\rm Zn}$ due to the absence of isobaric overlaps. Zinc also has a slightly increased ionization potential, so that ion yield is lower compared to other transition metals (e.g., Co). Whereas the element is limited in its reactivity to O2, a product ion is formed with NH3 through the addition of one molecule of NH3 per atom (e.g., $^{83}[^{66}{\rm Zn}({\rm NH}_3)]$). Higher amounts of sulfur present in a sample lead to the formation of $^{32}{\rm S}_2^{+}$ and $^{32}{\rm S}^{34}{\rm S}^{+}$, interfering on $^{64}{\rm Zn}$ and $^{66}{\rm Zn}$, which may be an issue in some environmental samples, such as waste waters or flow back solutions.

Element	Zinc	
Available isotopes	⁶⁴ Zn (48.60%), ⁶⁶Zn (27 ⁶⁸ Zn (18.80%),	
Ionization Potential	9.39 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Dreferred analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	$TQ-NH_3^{83}[66Zn(NH_3)]$

Gallium

Gallium has two stable isotopes, ⁶⁹Ga and ⁷¹Ga. The more abundant isotope can be seriously biased if the sample contains barium (the main isotope of barium is ¹³⁸Ba and tends to form ¹³⁸Ba⁺⁺ easily). Polyatomic interferences are less pronounced, although a significant overlap could be observed through ⁵⁵Mn¹⁴N⁺. Gallium can be applied as an internal standard.

Element	Gallium	
Available isotopes	⁶⁹ Ga (60.10%), ⁷¹ C	Ga (30.90%)
Ionization Potential	6.00 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Dreferred analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-NH ₃





Germanium is often used as a potential internal standard in a variety of applied applications, such as environmental analysis. Due to severe polyatomic and isobaric interferences on the major isotopes of germanium (e.g., ⁴⁰Ar³²S⁺ on ⁷²Ge, ⁷⁴Se⁺ on ⁷⁴Ge and Cl₂⁺ on both ⁷²Ge and ⁷⁴Ge), it is most commonly analyzed using a minor isotope, ⁷³Ge. If potential contributions from selenium can be excluded or are acceptably corrected through mathematical correction, ⁷⁴Ge is an appealing alternative due to its significantly higher abundance. Although the use of triple quadrupole technology would remove the isobaric interference of selenium on ⁷⁴Ge, the resulting sensitivity when using NH₃ is often lower as compared to KED. However, germanium is also an analyte of high interest in the semiconductor industry and therefore needs to be analyzed at very low levels in process chemicals, such as different acids or organic solvents. Often, the use of triple quadrupole technology is superior over cold plasma as germanium has a relatively high first ionization potential.

Element	Germanium	
Available isotopes	⁷⁰ Ge (20.50%), ⁷² Ge (27.40%), ⁷³ Ge (7.80%), ⁷ ⁷⁴ Ge (36.50%), ⁷⁶ Ge (7.80%)	
Ionization Potential	7.90 eV (15.94 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-NH ₃ (89[73Ge(14N1H ₂)]), TQ-O ₂ (73Ge)





Arsenic is monoisotopic at mass 75. Due to its toxicity, it is a mandatory element in many regulated methods. The most common interferences on arsenic are chlorine based, such as either ⁴⁰Ar³⁵Cl* or ⁴⁰Ca³⁵Cl*, which can be efficiently reduced using KED. Additional interferences such as ¹⁵⁰Nd* or ¹⁵⁰Sm* can be observed when rare earth elements are present. This is often the case for soil samples, but food samples are also likely to be affected. The optimal way to resolve these interferences is the use of oxygen in the collision / reaction cell (leading to the mass shift formation of ⁷⁵As¹⁶O*). Arsenic can also be present in a variety of different chemical forms, or species, varying dramatically in toxicity. The element is therefore a primary example for the need of speciation analysis in order to obtain information on the exact species present in a sample rather than the total concentration. Although potential interferences would be separated as well in the chromatographic separation, the use of triple quadrupole technolgy improves the overall sensitivity, enabling the detection of especially low abundant (and eventually otherwise missed) species.

Arsenic	
⁷⁵ As (100%)	
9.82 eV	
Intelligent Mass Selection (iMS)	
Reaction Finder Default	Alternatives
TQ-O ₂ (75As16O)	SQ-KED
	9.82 e Intelligent Mass Se Reaction Finder Default





Selenium has six stable isotopes with varying abundance. The most abundant isotope, 80 Se, is not the preferred choice due to the 40 Ar $_2^{\ +}$ interference derived from the argon plasma. On single quadrupole instruments, the preferred choice is therefore a less abundant, but less interfered isotope, such as 77 Se, 78 Se, or 82 Se. In addition, bromine can interfere on 80 Se and 82 Se through the formation of 79 Br'H $^{+}$ and 81 Br'H $^{+}$. Like arsenic, doubly charged ions of certain rare earth isotopes, such as 156,160 Gd, can cause doubly charged interferences on the main Se isotopes. As with arsenic, the optimal way to resolve these interferences is to use $\rm O_2$ in the cell to mass shift Se to SeO $^{+}$. This approach enables use of the most abundant 80 Se isotope, leading to drastically improved sensitivity and lower detection limits when using a triple quadrupole based ICP-MS instrument.

Selenium	
⁷⁴ Se (0.86%), ⁷⁶ Se (9.23%), ⁷⁷ Se (7.60%), ⁷⁸ Se (23.69%), ⁸⁰ Se (49.80%), ⁸² Se (8.82%)	
9.75 eV	
Intelligent Mass Selection (iMS)	
Reaction Finder Default	Alternatives
TQ-O ₂ (80Se16O)	SQ-KED (⁷⁸ Se), SQ-H ₂ (⁸⁰ Se)
	⁷⁴ Se (0.86%), ⁷⁸ Se (9.2 ⁷⁸ Se (23.69%), ⁸⁰ Se (49. 9.75 e Intelligent Mass S Reaction Finder Default



Bromine

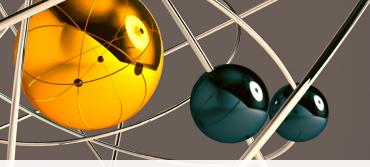
Like all halogens, bromine has a high 1st ionization potential, leading to low ion yield in an inductively coupled plasma. Nonetheless it can be analyzed with good detection limits. Bromine is even under regulation as it may form potentially carcinogenic BrO₂ as a byproduct in drinking water disinfection, requiring speciation analysis for separating other bromine containing species such as bromide (Br). Bromine has two equally abundant isotopes, which may only be interfered through polyatomic species in presence of high concentrations of transition metals such as copper (e.g., 63Cu¹⁶O+ and 65Cu¹⁶O+), or nickel (62Ni16O1H+ and 64Ni16O1H+). In addition, high concentrations of potassium may lead to the formation of 40Ar39K*, again interfering with the commonly analyzed isotope, ⁷⁹Br. In case the presence of rare earth elements is likely in a sample, the formation of doubly charged species of gadolinium (158Gd++), dysprosium (157 Dy++ and 158 Dy++) and erbium (162 Er++) may affect the detection of bromine. Because of the higher abundance of gadolinium among all rare earth elements, ⁷⁹Br is again likely more affected. However, because of its reactivity towards oxygen, all of the aforementioned interferences are safely removed using oxygen and a mass shift reaction. Bromine itself has the potential to interfere on ⁸⁰Se and ⁸²Se through the formation of hydrides (⁷⁹Br¹H⁺ and ⁸¹Br¹H⁺, respectively).

Element	Bromine	
Available isotopes	⁷⁹ Br (50.69%), ⁸¹ Br (49.31%)	
1st Ionization Potential	11.81 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Droformed analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	TQ-O ₂ (⁷⁹ Br ¹⁶ O)	SQ-KED, TQ-NH ₃ (⁷⁹ Br)









Rubidium

Rubidium is a typical alkali metal with low first ionization potential, but very high second ionization potential. None of its two isotopes is significantly interfered by polyatomic species, but its major isotope, ⁸⁵Rb, can be slightly positively biased when using scandium as an internal standard (formation of ⁴⁰Ar⁴⁵Sc⁺). The low reactivity of rubidium to O₂ (similar for all the alkali metals) can be used to resolve the potential isobaric overlap with ⁸⁷Sr, by enabling ⁸⁷Sr to be converted to SrO⁺ to move it away from ⁸⁷Rb.

Element	Rubidium	
Available isotopes	⁸⁵ Rb (72.17%), ⁸⁷ Rb (27.84%)	
Ionization Potential	4.18 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-O ₂ (⁸⁵ Rb), TQ-NH ₃ (⁸⁵ Rb)

Strontium

As with the majority of the alkaline earth elements, strontium forms a considerable amount of doubly charged ions and well as singly charged ions, leading to an interference on ^{44}Ca (through $^{88}\text{Sr}^{**}$). Out of its four isotopes, ^{89}Sr is usually applied for analysis. In geochemical analysis, the isotope ratio of $^{89}\text{Sr}/^{87}\text{Sr}$ is of interest for age determinations. However, ^{87}Rb creates an isobaric overlap, which can be removed through a mass shift reaction (forming $^{87}\text{Sr}^{16}\text{O*}$) using O₂. Other gases, such as N₂O or SF₆ have been described for this application as well, but are of limited use in a multi-element analysis.

Element	Strontium	
Available isotopes	84Sr (0.56%), 86Sr (9.86%), 87Sr (7.00%), 88Sr (82.58%)	
Ionization Potential	5.70 eV (11.03 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
Due fe use d'are d'are de c	Reaction Finder Default	Alternatives
Preferred analysis modes	TQ-O ₂ (88Sr ¹⁶ O)	SQ-KED

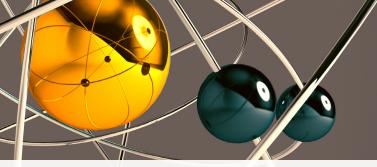
Yttrium

Yttrium is, like scandium or germanium, an element often recommended as an internal standard option in many regulatory methods. Typically, the formation of polyatomic interferences on its only isotope, ⁸⁹Y is rare, so that even standard mode (no interference removal) allows interference free detection.

Element	Yttrium	
Available isotopes	89 Y (100%)	
Ionization Potential	6.22 eV (12.23 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
Droformed analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	TQ-O ₂ (89Y16O)	SQ-KED, TQ-NH ₃ (89Y)







Zirconium

The main isotope, 90 Zr, makes up for more than half of all atoms of the element found in nature. Due to its unique properties, it is often applied in alloys and advanced materials, hence it will often be analyzed in combination with other metals, which may be interfered by its presence (e.g., palladium or silver). Zirconium is very reactive with O_2 , and readily forms higher oxides (such as ZrO_2^+ , ZrO_3^+) as well as ZrO^+ in the collision cell. This property is useful for removing ZrO^+ and $ZrOH^+$ interferences on Pd, Ag and Cd, which are not reactive towards oxygen.

Element	Zirconium	
Available isotopes	°Zr (51.45%), °Zr (11.22%), °Zr (17.15%), °Zr (17.38%), °Zr (2.80%)	
Ionization Potential	6.63 eV (13.16 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
Drafarrad analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	TQ-O ₂ (90Zr16O)	SQ-KED, TQ-NH ₃ (⁹⁰ Zr)

Niobium

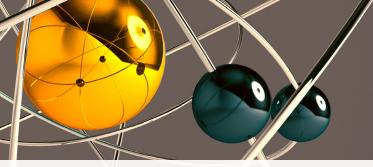
Niobium is monoisotopic at m/z 93. There are little polyatomic interferences to be expected under normal conditions, for example hydrides of zirconium or molybdenum (92 Zr₁H $^{+}$ and 92 Mo₁H $^{+}$), but also species of selenium formed in the plasma (e.g., 77 Se 16 O $^{+}$).

An overlap by doubly charged ions of tungsten, rhenium or osmium might be possible, but is unlikely based on the 2nd ionization potentials of these elements, all exceeding 16 eV (and therefore the ionization potential of argon) significantly. Niobium reacts with oxygen in a mass shift reaction and can therefore be easily analyzed free from interferences using a triple quadrupole ICP-MS. It forms also some product ions with ammonia, but the on mass reaction is typically providing a better sensitivity.

Element	Niobium	
Available isotopes	⁹³ Nb (100%)	
1st Ionization Potential	6.76 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
	Reaction Finder Default	Alternatives
Preferred analysis modes	TQ-O ₂ (93Nb16O)	SQ-KED, TQ-NH ₃ (93Nb)







Molybdenum

Molybdenum has a number of stable isotopes between m/z 92 and m/z 100. Although potentially interfered by several oxides, nitrides or argides formed by other elements, all of these interferences can be efficiently reduced using KED. It is reactive with oxygen and can be analyzed via a mass shift process. This is used to remove molybdenum based interferences on cadmium. Similar to zirconium, molybdenum is also very reactive to oxygen and forming higher oxides.

Element	Molybdenum	
Available isotopes	⁹² Mo (14.84%), ⁹⁴ Mo (9.25%), ⁹⁵ Mo (15.92%), ⁹⁶ Mo (16.68%), ⁹⁷ Mo (9.55%), ⁹⁸ Mo (24.13%), ¹⁰⁰ Mo (9.63%)	
Ionization Potential	7.09 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Duafawa di analysia mada	Reaction Finder Default	Alternatives
Preferred analysis modes	TQ-O ₂ (98 Mo ¹⁶ O)	SQ-KED

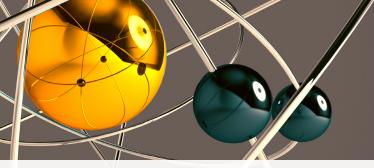
Silver

Silver is increasingly being used in the production of nanomaterials with antibacterial properties in a variety of consumer products. This is leading to an increase of the amount of silver found in the environment, mostly in its ionic form Ag $^{+}$, but also as nanomaterial. Although its two isotopes are almost equally abundant, 107 Ag is the preferred isotope for analysis. Silver is potentially interfered when metals such as zirconium or niobium are present. These elements form oxide (93 Nb 16 O interfering on 109 Ag) and hydroxide ions (90 Zr 16 O 1 H interfering on 107 Ag), which can be efficiently removed using O $_{2}$. Silver is not reactive with O $_{2}$ due to its noble chemical nature, and so the above interferences can be further oxidized and hence mass separated.

Element	Silver	
Available isotopes	¹⁰⁷ Ag (51.84%), ¹⁰⁹ Ag (48.16%)	
Ionization Potential	7.58 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Preferred analysis modes	Reaction Finder Default	Alternatives
Freierred analysis modes	SQ-KED	TQ-O ₂ (107Ag)







Cadmium

Cadmium has a total of eight stable isotopes. Although <code>ii4Cd</code> has the highest abundance, the preferred choice in ICP-MS is usually <code>ii1Cd</code> due to the absence of isobaric overlaps with isotopes of palladium or tin, which affect all other isotopes of Cd. The most prominent interference on <code>ii1Cd</code> is caused through <code>95Mo16O+</code>, but also zirconium can interfere (<code>94Zr16O1H+</code>). As cadmium is not reactive towards O_2 , an oxidation reaction of molybdenum (forming predominantly <code>95Mo16O_2+</code>) can be used in an on mass measurement.

Element	Cadmium	
Available isotopes	¹⁰⁶ Cd (1.25%), ¹⁰⁶ Cd (0.89%), ¹¹⁰ Cd (12.49%), ¹¹¹ Cd (12.80%), ¹¹² Cd (24.13%), ¹¹³ Cd (12.22%), ¹¹⁴ Cd (28.73%), ¹¹⁶ Cd (12.49%)	
Ionization Potential	8.99 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-O ₂ (111 Cd)

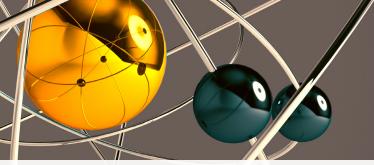
Indium

Indium is the only element in the Periodic Table that has no isotope free from isobaric overlap. Both isotopes, ¹¹³In and ¹¹⁵In, are interfered through other isotopes of either cadmium or tin. However, the abundance of ¹¹³In is significantly lower compared to ¹¹⁵In, so that only the latter isotope is used for analysis. Indium is commonly used as an internal standard, but mathematical correction for Cd or Sn interference is feasible to avoid negative impact on the results, since polyatomic interferences or contributions of doubly charged ions are unlikely. Indium shows no significant reactivity to O₂, NH₃ or H₂, so that all measurement modes will be on mass.

Element	Indium	
Available isotopes	¹¹³ In (4.30%), ¹¹⁵ In (95.70%)	
Ionization Potential	5.79 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-O ₂ (¹¹⁵ In), TQ-NH ₃ (¹¹⁵ In)







Tin

Tin is the element with the highest number of stable isotopes found in the Periodic Table with a total of 10 isotopes. Tin therefore causes a significant number of isobaric overlaps, which can in most cases be accounted for by using mathematical corrections. For ICP-MS analysis, there are two isotopes which are recommended for analysis, ¹¹⁸Sn and ¹²⁰Sn, as these are the most abundant isotopes. Both are free from isobaric overlaps through other elements and little affected by polyatomic interferences in the most typical sample matrices. Tin is commonly analyzed using kinetic energy discrimination. It shows no significant reactivity towards the commonly used reactive gases.

Element	Tin	
Available isotopes	¹¹² Sn (0.97%), ¹¹⁴ Sn (0.6 ¹¹⁶ Sn (14.53%), ¹¹⁷ Sn (7.6 ¹¹⁹ Sn (8.58%), ¹²⁰ Sn (32. ¹²⁴ Sn (5.7	8%), ¹¹⁸ Sn (24.22%), 59%), ¹²² Sn (4.63%),
Ionization Potential	7.34 eV (14.63 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
Drafarrad analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-NH ₃ (118, 120Sn)

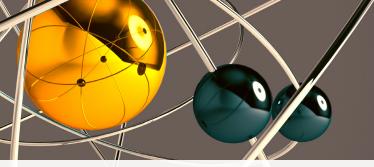
Antimony

Antimony has two isotopes with similar abundance, and both are equally suitable for ICP-MS analysis. The use of kinetic energy discrimination is mostly sufficient for analysis, as polyatomic interferences will only be formed in the presence of certain elements, such as silver or palladium (as oxides or nitrides). Like tin, antimony does not show reactivity to either O_2 , H_2 , or NH_3 .

Element	Antimony	
Available isotopes	¹²¹ Sb (57.30%), ¹²	°Sb (42.70%)
Ionization Potential	8.64 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Dreferred analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-NH ₃ (121Sb)







Tellurium

Tellurium is an element occasionally used as an internal standard, but is also becoming more important for analysis in environmental studies in order to better understand its toxicity and pathways as a contaminant. As a non-metal, it's ionization potential is high, limiting the ion yield, and its most abundant isotopes are interfered by isobaric overlaps of xenon (128 Xe on 128 Te, having an abundance of 31.69%), and more importantly barium on the most abundant isotope 130 Te (with an abundance of 33.80%). However, using $\rm O_2$ as a reactive gas, xenon ions are efficiently removed from the ion beam, whereas barium ions undergo an oxidation and are hence separated in the analyzing quadrupole after reaction. Tellurium can therefore be detected interference free using the most abundant isotope with triple quadrupole ICP-MS, whereas less abundant 125 Te would be the common choice on a single quadrupole instrument.

Element	Tellurium	
Available isotopes	¹²⁰ Te (0.10%), ¹²² Te (2.60%), ¹²³ Te (0.91%), ¹²⁴ Te (4.82%) ¹²⁵ Te (7.14%), ¹²⁶ Te (18.95%), ¹²⁶ Te (31.69%), ¹³⁰ Te (33.80%)	
Ionization Potential	9.01 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Due fe weed even by single ended	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-O ₂ (130Te)

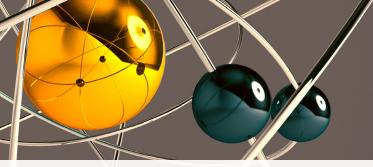
lodine

lodine is monoisotopic in nature (127 I), but has a few artificial isotopes, such as 129 I or 131 I, which are of analytical interest. These isotopes are long-lived therefore subject to environmental forensic analysis. Due to the presence of Xe as a common impurity in argon gas, there is an isobaric interference on both 129 I and 131 I, which can be removed using O_2 . Moreover, if trace analysis of 129 I next to high amounts of natural iodine is required, significant backgrounds can be formed through the formation of 127 I 11 H $_2$, which can be reduced using triple quadrupole instrumentation.

Element	lodine	
Available isotopes	127 (100%), artificial isotopes 129 and 131	
Ionization Potential	10.45 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Preferred analysis modes	Reaction Finder Default	Alternatives
Freierred analysis modes	SQ-KED	TQ-O ₂ (127)







Cesium

Cesium is monoisotopic at m/z 133, but has long-lived artificial isotopes, such as 137 Cs, which are of interest in environmental forensics. Whereas 133 Cs shows no significant interferences, 137 Cs is interfered through an isobaric overlap with 137 Ba. In order to separate the elements from each other, O_2 can be applied, leading to a mass shift reaction of Ba and hence interference removal.

Element	Cesium	
Available isotopes	¹³³ Cs (100%), artificial isotope ¹³⁷ Cs	
Ionization Potential	3.89 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Drafarrad analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-O ₂ (133Cs)

Barium

Barium is abundant in nature and has a total of 7 isotopes. For the quantitative analysis of barium either $^{\rm 137}{\rm Ba}$ or $^{\rm 138}{\rm Ba}$ are applied (using SQ-KED or TQ-O $_{\rm 2}$ mode), but the other minor isotopes need to be considered as potential interferences on other elements, such as tellurium or cesium. Due to its low second ionization potential, barium is a likely interference on elements such as gallium through the formation of doubly charged ions.

Element	Barium	
Available isotopes	¹³⁰ Ba (0.11%), ¹³² Ba (0.10%), ¹³⁴ l ¹³⁸ Ba (7.85%), ¹³⁷ Ba (11.2	
Ionization Potential	5.21 eV (10.00 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
Preferred analysis modes	Reaction Finder Default	Alternatives
Freierred analysis modes	SQ-KED	TQ-O ₂ (138Ba16O)



Rare Earth Elements

The rare earth elements comprise a group of 14 elements (from lanthanum to lutetium) in the mass range between 139 and 176. Because of their high chemical similarity, these elements often occur in combination with each other, the most abundant single element out of the series being gadolinium. An exception is promethium, which does not occur naturally and is not included here. All rare earth elements are characterized by a low 1st ionization potential (yielding a high detection sensitivity at normally low backgrounds), but also a moderate 2nd ionization potential, leading to a variety of potentially occurring doubly charged interferences. Furthermore, all rare elements tend to form stable oxides, so that although there is an isotope free from isobaric overlaps for each element, these polyatomic interferences can be of concern when measuring heavier rare earth elements in presence of their lower mass homologues. This is especially obvious for the determination of ytterbium in the presence of gadolinium. Both elements have an identical number of isotopes with almost identical abundances, but exactly 16 mass units apart. Therefore, the presence of gadolinium makes the determination of ytterbium at low levels very difficult. However, these elements also show different reactivities towards NH₂, so that resolution of the aforementioned interferences is possible using triple quadrupole ICP-MS. Elements such as Pr, Eu, Dy, Ho, Er, Tm and Yb do not (or only to a negligible extent) react with NH₂, but oxide interferences are effectively removed. The remaining elements, La, Ce, Nd, Sm, Gd, Tb and Lu do react with NH₃, but less effectively compared to the reaction with O₂. Often, a reaction with O2 (and hence the formation of the MO+ product ion) is the preferred choice. Element descriptions follow on next pages.

Element	Lanthanum	
Available isotopes	¹³⁸ La (0.09%), ¹³⁹ La (99.91%)	
Ionization Potential	5.58 eV (11.06 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
Dueferus de cachacie accedes	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-O ₂ (139La16O)
Element	Cerium	
Available isotopes	¹³⁶ Ce (0.19%), ¹³⁸ Ce (0.25%), ¹⁴⁰ Ce (88.48%), ¹⁴² Ce (11.08%	
Ionization Potential	5.54 eV (10.	88 eV)
Q1 resolution	Intelligent Mass Selection (iMS)	
Droforrad analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	TQ-O ₂ (140 Ce ¹⁶ O)	SQ-KED
Element	Praseodymium	
Available isotopes	¹⁴¹ Pr (100%)	
Ionization Potential	5.46 eV (10.57 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
Dueferused exelusions also	Reaction Finder Default	Alternatives
Preferred analysis modes	TQ-O ₂ (141Pr16O)	SQ-KED

Additional element descriptions follow on next page.





Rare Earth Elements continued

Element	Neodymium	
Available isotopes	¹⁴² Nd (27.13%), ¹⁴³ Nd (12.18%), ¹⁴⁴ Nd (23.80%), ¹⁴⁵ Nd (8.30%), ¹⁴⁶ Nd (17.19%), ¹⁴⁸ Nd (5.76%), ¹⁵⁰ Nd (5.64%)	
Ionization Potential	5.53 eV (10.78 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
	Reaction Finder Default	Alternatives
Preferred analysis modes	TQ-O ₂ (144Nd16O)	SQ-KED
Element	Samarium	
Available isotopes	¹⁴⁴ Sm (3.10%), ¹⁴⁷ Sm (15.00%), ¹⁴⁸ Sm (11.30%), ¹⁴⁹ Sm (13.80%), ¹⁵⁰ Sm (7.40%), ¹⁵² Sm (26.70%), ¹⁵⁴ Sm (22.70%)	
Ionization Potential	5.64 eV (11.09 eV)	
Q1 resolution	Intelligent Mass Sel	ection (iMS)
Duefermed en alveia de ade	Reaction Finder Default	Alternatives
Preferred analysis modes	TQ-O ₂ (149 Sm ¹⁶⁰)	SQ-KED
Element	Europium	
Available isotopes	¹⁵¹ Eu (47.80%), ¹⁵³ Eu (52.20%)	
Ionization Potential	5.67 eV (11.25 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
Duefermed and hade made	Reaction Finder Default	Alternatives
Preferred analysis modes	SO-KED	TO_O (153Fu)

SQ-KED

Element	Gadolinium	
Available isotopes	¹⁵² Gd (0.20%), ¹⁵⁴ Gd (2.18%), ¹⁵⁵ Gd (14.80%), ¹⁵⁶ Gd (20.47%), ¹⁵⁷ Gd (15.65%), ¹⁵⁸ Gd (24.84%), ¹⁶⁰ Gd (21.86%)	
Ionization Potential	6.15 eV (12.13 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
Duefe weed as a business day	Reaction Finder Default	Alternatives
Preferred analysis modes	TQ-O ₂ (157Gd16O)	SQ-KED
Element	Terbium	
Available isotopes	¹⁵⁹ Tb (100%)	
Ionization Potential	5.86 eV (11.50 eV)	
Q1 resolution	Intelligent Mass Se	lection (iMS)
Due ferme di cue el mele une el de	Reaction Finder Default	Alternatives
Preferred analysis modes	TQ-O ₂ (159Tb16O)	SQ-KED
Element	Dysprosi	um
Available isotopes	¹⁵⁶ Dy (0.06%), ¹⁵⁸ Dy (0.10%), ¹⁶⁰ Dy (2.34%), ¹⁶¹ Dy (18.90%), ¹⁶² Dy (25.50%), ¹⁶³ Dy (24.90%), ¹⁶⁴ Dy (28.20%)	
Ionization Potential	5.94 eV (11.71 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
Dreferred analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	TQ-O ₂ (163 Dy 16 O)	SQ-KED

Additional element descriptions follow on next page.



TQ-O₂ (153 Eu)



Rare Earth Elements continued

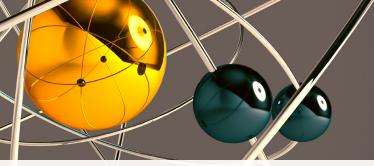
Element	Holmium	
Available isotopes	¹⁶⁵ Ho (100%)	
Ionization Potential	6.02 eV (11.82 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
Drafarrad analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes -	TQ-O ₂ (165Ho16O)	SQ-KED
Element	Erbium	
Available isotopes	¹⁶² Er (0.14%), ¹⁶⁴ Er (1.61%), ¹⁶⁶ Er (33.60%), ¹⁶⁷ Er (22.95%), ¹⁶⁸ Er (26.80%), ¹⁷⁰ Er (14.90%)	
Ionization Potential	6.10 eV (11.92 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
Droformad analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes -	TQ-O ₂ (166Er16O)	SQ-KED
Element	Tullium	
Available isotopes	¹⁶⁹ Tm (100%)	
Ionization Potential	6.18 eV (12.02 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
Professed analysis medes	Reaction Finder Default	Alternatives
Preferred analysis modes -	TQ-O ₂ (169Tm16O)	SQ-KED

Element	Ytterbium	
Available isotopes	¹⁶⁸ Yb (0.13%), ¹⁷⁰ Yb (3.05%), ¹⁷¹ Yb (14.30%), ¹⁷² Yb (21.90%), ¹⁷³ Yb (16.12%), ¹⁷⁴ Yb (31.80%), ¹⁷⁶ Yb (12.70%)	
Ionization Potential	6.25 eV (12.18 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
Duefermed engliseie meedee	Reaction Finder Default	Alternatives
Preferred analysis modes —	SQ-KED	TQ-O ₂ (172Yb)
Element	Lutetium	
Available isotopes	¹⁷⁵ Lu (97.41%), ¹⁷⁶ Lu (2.59%)	
Ionization Potential	5.43 eV (13.89 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
Droforrad analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes —	TQ-O ₂ (175Lu ¹⁶ O)	SQ-KED









Hafnium

Hafnium is rarely of interest for quantitation, however, Hf isotopes can be relevant in geosciences for the determination of the petrogenesis of igneous rocks, and can be used to show crust or mantle mixing and weathering cycles. However, there are isobaric overlaps caused by ytterbium and tungsten on some of the key isotopes, which can be removed using NH₃. Whereas ytterbium is close to unreactive to this gas, a variety of cluster ions are formed with hafnium, mostly following the general formula [Hf(NH₂)(NH₃)x], the most abundant one being [Hf(NH₂)(NH₃)₃]*. Other rare earth elements, potentially more reactive towards NH₃, are efficiently removed in the first quadrupole.

For quantitative analysis, the selection of TQ-O₂ mode using ¹⁷⁸Hf is a viable way of assuring full interference removal and increasing the detection sensitivity.

Element	Hafnium	
Available isotopes	¹⁷⁴ Hf (0.16%), ¹⁷⁶ Hf (5.21%), ¹⁷⁷ Hf (18.61%), ¹⁷⁸ Hf (27.30%), ¹⁷⁹ Hf (13.63%), ¹⁸⁰ Hf (35.10%)	
Ionization Potential	6.83 eV (14.93 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
Dreferred analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	TQ-O ₂ (178Hf16O)	TQ-NH ₃ (178[NH(NH ₂)(NH ₃) ₃)]

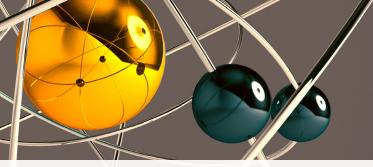
Tantalum

Tantalum is quasi-monoisotopic, as its major isotope, ¹⁸¹Ta, has an abundance of 99.99%. Tantalum is one of the rarest elements on earth, but is used in a variety of applications, from electronic components to medical implants. Therefore, it is not commonly analyzed. The only relevant polyatomic interferences can be formed with rare earth elements, for example ¹⁶⁵Ho¹⁶O⁺, if Ho is present in the sample. However, Ta reacts efficiently with oxygen, so that formation of ¹⁸¹Ta¹⁶O is a good way of eliminating the aforementioned Ho interference.

Element	Tantalum	
Available isotopes	¹⁸⁰ Ta (0.01%), ¹⁸¹ Ta (99.99%)	
Ionization Potential	7.89 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Dreferred analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	TQ-O ₂ (181Ta16O)	SQ-KED, TQ-NH ₃ (181Ta)







Tungsten

Tungsten has a total of five stable isotopes, of which ¹⁸²W is the most common choice for analysis. As is generally the case in the high mass range, polyatomic interferences on W are rare, so that in most cases, only isobaric overlaps are considered. Some isotopes of tungsten may be affected by oxide ions of less abundant rare earth elements, such as thulium or erbium. Tungsten itself may be found as an interference on mercury, especially through its major isotopes ¹⁸⁴W and ¹⁸⁶W (interfering as WO+ or WOH+ ions).

Element	Tungsten	
Available isotopes	¹⁸⁰ W (0.13%), ¹⁸² W (26.30%), ¹⁸³ W (14.30%), ¹⁸⁴ W (30.67), ¹⁸⁶ W (28.60%)	
Ionization Potential	7.98 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	$TQ-NH_3$ (265[182W(14N1H)(14N1H3)4)]

Rhenium

Rhenium is occasionally used as an internal standard due its rare occurrence in nature, mostly using its minor isotope ¹⁸⁵Re, which is not affected by isobaric overlaps.

Element	Rhenium	
Available isotopes	¹⁸⁵ Re (37.40%), ¹⁸⁷ Re (62.60%)	
Ionization Potential	7.88 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-O ₂ (¹⁸⁵ Re), TQ-NH ₃ (¹⁸⁵ Re)







Ruthenium

Ruthenium is commonly determined using the third most abundant of its seven stable isotopes, $^{\tiny 101}\text{Ru}$. Other isotopes, such as the most abundant $^{\tiny 102}\text{Ru}$ are affected by isobaric overlaps. Typically, there are almost no polyatomic interferences affecting the detection of $^{\tiny 101}\text{Ru}$, so that even standard mode (CRC used as an ion guide only) would provide accurate results. As with all platinum group metals, ruthenium is not reactive to O_2 , but slightly reactive to NH_3 , forming a cluster ion through the addition of one NH_3 molecule per atom.

Element	Ruthenium	
Available isotopes	⁹⁶ Ru (5.52%), ⁹⁶ Ru (1.88%), ⁹⁶ Ru (12.70%), ¹⁰⁶ Ru (12.60%), ¹⁰¹ Ru (17.00%), ¹⁰² Ru (31.60%), ¹⁰⁴ Ru (18.70%)	
Ionization Potential	7.36 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Preferred analysis modes	Reaction Finder Default	Alternatives
	SQ-KED	SQ-N/A

Rhodium

Rhodium is monoisotopic with its only isotope being 103 Rh. It is often analyzed in order to assess purity of metals or metal alloys and can be interfered in the presence of high concentrations of Cu (63 Cu 40 Ar') and lead (206 Pb $^{++}$). Whereas the copper based interference can be effectively removed using KED, the lead induced interference can only be removed using O_2 as a reactive gas, in which case, 103 Rh will be determined on mass. Due to the frequent use of rhodium as an internal standard, interferences caused by higher concentrations of lead can be misinterpreted as an unexplained matrix effect.

Element	Rhodium	
Available isotopes	¹º³Rh (100%)	
Ionization Potential	7.46 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Duefe weed available made	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-O ₂ (103Rh)





Platinum Group Metals (PGMs)

Palladium

Palladium has a series of isotopes, the default selection often being $^{105}{\rm Pd}$ due to the absence of isobaric overlaps (caused by either ruthenium or cadmium). However, since $^{89}{\rm Y}$ is an element often used as an internal standard, there may be elevated backgrounds or false positive results observed through the formation of $^{89}{\rm Y}^{16}{\rm O}^*$. Like most PGMs, Pd is unreactive towards ${\rm O}_2$ and can be analyzed interference free on mass.

Element	Palladium	
Available isotopes	¹⁰² Pd (1.02%), ¹⁰⁴ Pd (11.14%), ¹⁰⁵ Pd (22.33%), ¹⁰⁶ Pd (27.33%), ¹⁰⁸ Pd (26.46%), ¹¹⁰ Pd (11.72%)	
Ionization Potential	8.34 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Duefe weed an alvais was dee	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-O ₂ (105Pd)

Osmium

Osmium has a total of 7 stable isotopes, but despite the high number, $^{\tiny 192}\text{Os}$ still shows a reasonable abundance of 41.00%. However, due to isobaric interferences with $^{\tiny 192}\text{Pt}$, the preferred isotope for analysis is often $^{\tiny 189}\text{Os}$. Due to a similar reactivity of Pt and Os towards both O_2 and NH $_3$, the selection of this alternative isotope is the best option. Osmium is well known to be affected by physical interferences and losses occurring during sample preparation and analysis, especially because of its high volatility in its oxidized form (e.g., after a microwave digestion). As well as potentially being lost to the atmosphere on opening the digestion vessel, Os can also be volatilized preferentially in the spray chamber, which may lead to an overestimation when not calibrated using standards containing the same chemical form of Os.

Element	Osmium	
Available isotopes	¹⁸⁴ Os (0.02%), ¹⁸⁶ Os (1.58%), ¹⁸⁷ Os (1.60%), ¹⁸⁸ Os (13.30%), ¹⁸⁹ Os (16.10%), ¹⁹⁰ Os (26.40%), ¹⁹² Os (41.00%)	
Ionization Potential	8.71 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-O ₂ (189Os), TQ-NH ₃ (204[189Os(14N1H)])







Iridium

Like all platinum group metals, iridium is analyzed as part of the composition and impurity analysis of ores and refined metals/alloy products. Iridium is also often used as a high mass internal standard. Its more abundant mass 193 isotope (193 Ir) may be interfered by oxide or hydroxide ions of elements such as lutetium and hafnium, but by itself it can create an oxide interference on 209 Bi. Similar to the aforementioned elements, interferences can be removed through the use of O_9 , to which Ir shows only limited reactivity.

Element	Iridium	
Available isotopes	¹⁹¹ lr (37.30%), ¹⁹³ lr (62.30%)	
Ionization Potential	9.12 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Drafarrad analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-O ₂ (193 lr)

Platinum

The two most abundant isotopes of platinum are $^{\tiny 194}\text{Pt}$ and $^{\tiny 195}\text{Pt}$ (with 32.90 and 33.80% relative abundance), however, both may be interfered through hafnium oxide and hydroxide interferences. On mass measurements using O $_2$ cell gas are an effective way to remove these interferences. In contrast to other platinum group metals, platinum also forms product ions with NH $_3$, such as $^{\tiny 229}[^{\tiny 195}\text{Pt}(\text{NH}_3)_2]^*$.

Element	Platinum	
Available isotopes	¹⁹⁰ Pt (0.01%), ¹⁹² Pt (0.79%), ¹⁹⁴ Pt (32.90%), ¹⁹⁵ Pt (33.80%), ¹⁹⁶ Pt (25.30%), ¹⁹⁸ Pt (7.20%)	
Ionization Potential	9.02 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-O ₂ (195Pt) or TQ-NH ₃ (229[195Pt(NH ₃) ₂])







Gold

Gold is often used for stabilization and reduction of memory effects of mercury, commonly during the analysis of environmental samples (drinking waters or waste waters), food samples or pharmaceutical products. In recent years, it has started to be used in nanomaterial production and can therefore also be found increasingly in the environment. Gold is an important analyte for the assessment of the content or impurity levels in ores and metals/alloys, where its only isotope 197 Au can be interfered by 181 Ta 16 O $^{\circ}$. The determination of gold in materials containing platinum may be affected through hydride formation and peak tailing of the 196 Pt and 198 Pt isotopes, which can be reduced through the use O_2 in the collision cell in combination with high mass resolution on the analyzing quadrupole. Like platinum, cluster ions of identical composition can be formed with NH $_2$ as a reactive gas.

Element	Gold	
Available isotopes	¹⁹⁷ Au (100%)	
Ionization Potential	9.23 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-O $_2$ (197Au) or TQ-NH $_3$ (231[197Au(NH $_3$) $_2$])

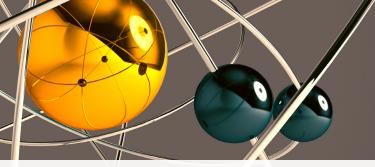
Mercury

Mercury is a key element in many regulated methods due to its elevated toxicity. Out of its seven stable isotopes, commonly the most abundant ²⁰²Hg is applied for analysis. Occasionally, interferences caused through the presence of tungsten (forming for example ¹⁸⁶W¹⁶O*) can be found to bias results. Similar to the removal of molybdenum interferences on cadmium, O₂ can be used to convert WO* species into WO₂* derivatives, whereas mercury is not reactive and can be determined interference free on mass.

Element	Mercury	
Available isotopes	¹⁹⁶ Hg (0.14%), ¹⁹⁸ Hg (10.02 ²⁰⁰ Hg (23.13%), ²⁰¹ Hg (13.22 ²⁰⁴ Hg (6.8	2%), ²⁰² Hg (29.80%),
Ionization Potential	10.44 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Drafarrad analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-O ₂ (²⁰² Hg)







Thallium

Thallium is a highly toxic metal, having two isotopes, which can normally considered interference free. It shows limited reactivity to both O₂ and NH₃, but formation of product ions is less favorable compared to measuring unreacted TI.

Element	Thallium	
Available isotopes	²⁰³ TI (29.52%), ²⁰⁵ TI (70.48%)	
Ionization Potential	6.11 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Drafarrad analysis mades	Reaction Finder Default	Alternatives
Preferred analysis modes	SQ-KED	TQ-O ₂ , TQ-NH ₃ (²⁰⁵ TI)

Lead

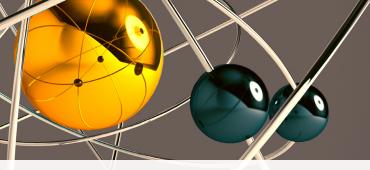
Lead is an exception in the Periodic Table as its isotopic composition may vary considerably in different regions. This is because three out of the four stable Pb isotopes are formed through radioactive decay of uranium or thorium. It is common practice to calculate the sum of all isotopes rather than using the result of a single isotope for quantitation. The use of KED mode is the method of choice, as polyatomic interferences are seldomly observed for lead. An exception is the determination of lead isotope ratios, which is of high interest in geosciences. The variable formation of ²⁰⁶Pb, ²⁰⁷Pb and ²⁰⁸Pb is a well-accepted way to determine the age of a rock. However, the ²⁰⁴Pb isotope (the only one not formed through radioactive decay) has an isobaric interference from ²⁰⁴Hg. Whereas a single quadrupole ICP-MS would have to rely on mathematical correction, triple quadrupole ICP-MS systems can fully eliminate the interference using NH₃. Whereas lead is not reactive to NH₃, Hg is efficiently removed.

Element	Lead	
Available isotopes	²⁰⁴ Pb (1.40%), ²⁰⁶ Pb (24.10%), ²⁰⁷ Pb (22.10%), ²⁰⁸ Pb (52.40%)	
Ionization Potential	7.42 eV (15.03 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
Preferred analysis modes	Reaction Finder Default	Alternatives
	SQ-KED	TQ-NH ₃ (²⁰⁴⁻²⁰⁸ Pb)









Bismuth

Bismuth is monoisotopic and often used as an internal standard for heavy elements such as lead or mercury. It is normally not interfered and unreactive to the common gases $\rm O_2$, $\rm NH_3$ and $\rm H_2$. However, it can be present as an impurity in some samples.

Element	Bismuth	
Available isotopes	²⁰⁹ Bi (100%)	
Ionization Potential	7.29 eV	
Q1 resolution	Intelligent Mass Selection (iMS)	
Preferred analysis modes	Reaction Finder Default	Alternatives
	SQ-KED	TQ-O ₂ , TQ-NH ₃ (²⁰⁹ Bi)

Thorium, Uranium

Both these elements are only still present in nature because of the extremely long half-lives of some of their isotopes. Other isotopes may exist as decay products, but are often short lived and hence not relevant for quantitative assessment. For thorium, the ²³²Th isotope is the most stable, having a halflife of around 14 billion years. It is essentially monoisotopic in practice, but detectable levels of 230Th (with a half-life of 75 thousand years) have been found in deep ocean waters and sediments. For uranium the 298U isotope (with a half-life of 4.5 billion years) has the highest mass and also the highest natural abundance of all U isotopes. The second most abundant isotope, ²³⁵U, has a half-life of 700 million years. Due to their low ionization potential, both elements can be measured with high ion yield and hence high sensitivity. For uranium, the use of O₂ and subsequent conversion into ²³⁸U¹⁶O₂⁺ is an option to improve sensitivity even further. Uranium can cause peak tailing onto adjacent masses (especially m/z 237 and 239), but the use of triple quadrupole technology also allows the impact of this tailing to be significantly reduced by mass filtration in Q1 and Q3 respectively, as well as by differential reactivity of isotopes such as ²³⁷Np and ²³⁹Pu towards O₂.

Element	Thorium	
Available isotopes	²³² Th (100%), half life 1.405 x 10 ¹⁰ years	
1st Ionization Potential	6.08 eV (11.50 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
Preferred analysis modes	Reaction Finder Default	Alternatives
	SQ-KED	TQ-O ₂ (²³² Th)
Element	Uranium	
Available isotopes	²³⁴ U (0.01%), ²³⁵ U (0.72%), ²³⁸ U (99.27%) half live between 2.5 x 10 ⁵ and 4.5 x 10 ⁹ years	
Ionization Potential	6.19 eV (14.72 eV)	
Q1 resolution	Intelligent Mass Selection (iMS)	
Preferred analysis modes	Reaction Finder Default	Alternatives
	SQ-KED	TQ-O ₂ (²³⁸ U ¹⁶ O ₂)



Conclusion

The use of triple quadrupole ICP-MS offers new possibilities for the analysis of elemental contaminants. Whereas for some elements, the default selection of an analysis mode assuring full interference removal and best limits of detection is not different between single and triple quadrupole instruments, there are significant differences for a variety of other elements. In these cases, the use of triple quadrupole technology allows all types of interferences—polyatomic, doubly charged ions and isobaric interferences—to be removed. In addition, the use of reactive gases in combination with suitable bias settings between the CRC and analyzing quadrupole allows the achievable sensitivity, and hence the detection limits, to be significantly improved. The use of triple quadrupole technology therefore allows analysis performance to be enhanced, although interference removal may not always be an issue for all elements.

At the same time, for a large variety of elements, effective interference removal can be accomplished through the combination of only two measurement modes, SQ-KED and TQ-O2, so that even in high throughout analysis demanding routine laboratories, the added time per sample will only be in the order of a few seconds to accommodate the gas exchange between helium and oxygen. For advanced applications, or special interference challenges, the use of ammonia can be an attractive alternative, not only to allow highly selective and specific interference removal, but also to provide a further improvement of detection sensitivity.



