High Resolution
Multicollector Mass Spectrometers
Based on more than 25 years experience in variable multicollector instrumentation, we have developed two instruments based on an innovative multicollector platform.

- High resolution ion optics corrected for second order image aberrations
  - Largest mass dispersion (812 mm)
  - Angular and energy focusing image planes are almost coincident
- Zoom optics to enhance dynamic multicollector measurements
  - Precise peak overlap for multi-dynamic measurements
- Field proven Faraday cups with largest aspect ratio
  - No cup factors
- Multiple Ion Counting (MIC)
  - Up to 8 moveable miniaturized SEMs in parallel
- Variable multicollector
  - Variable in position
  - Variable in detector type (Faraday/SEM)
  - Up to 17 collectors in parallel
  - “Plug-in” design of Faradays and SEMs
  - 17% relative mass range
- Virtual Amplifier system
  - No amplifier calibration bias
  - Linear response up to 50 V (positive ion mode)
- 10 kV acceleration voltage
  - Highest sensitivity
- All metal-sealed vacuum system
  - Ultra high vacuum system
  - High abundance sensitivity
  - Bakeable at high temperature
- Retardation lens (RPQ option)
  - Excellent abundance sensitivity
- Single focusing for thermal ionization source
  - Thermo Scientific TRITON
- Double focusing for inductively coupled plasma source
  - Thermo Scientific NEPTUNE
No Compromise
is the common philosophy
Thermo Scientific TRITON

The Thermo Scientific TRITON sets standards in high precision TIMS isotope ratio measurements. Its unique capabilities have earned it the reputation of the "natural choice" in TIMS instrumentation.

- Guaranteed external precision of Nd and Sr is 5 ppm (1 SD), both in static and multi-dynamic acquisition
- 2 ppm external precision has been shown
- Improved sensitivity
- 21 position sample turret for high throughput
- User friendly software with network capabilities
The Thermo Scientific NEPTUNE completes our integrated product family for elemental and isotopic analysis. It shares the field proven ICP interface with the Thermo Scientific ELEMENT 2, the most advanced single collector high mass resolution ICP-MS. The NEPTUNE and the TRITON are using the same high precision multicollector platform.

The NEPTUNE defines a “third generation” Multicollector ICP-MS, combining, for the first time, the features of high mass resolution, variable multicollection, zoom optics and multiple ion counting (MIC).

• High mass resolving power with flat top peak sections
• Excellent short-term and long-term stability of signal intensity and mass bias
• Full sensitivity with standard sample introduction system
• Fully integrated software for unattended operation and high throughput
Key Technologies

Advanced Multicollector Ion Optics

Large mass dispersion using an ion optical magnification of 2:
The large mass dispersion of 812 mm provides generous space for the versatile collector array. The mass dispersion is achieved by an ion optical magnification of 2, which has the additional advantages of increased focal depth and improved cup performance.

High Performance Faraday Cups

The Faraday cups are the largest ever produced for a commercial multicollector. They are laser machined from solid carbon to guarantee uniform response, high linearity, low noise and long lifetime. The Faraday cups are designed to completely eliminate the need for cup factors.1

The effect of ion optical magnification on cup performance is depicted in the figure. With increasing ion optical magnification the divergence angles of the ion beams are reduced and the dispersion is increased. As a result, cups can be wider and deeper. Scattered particles released at the cup’s side wall by the incoming ion beams are less likely to escape and do not alter the “true” ion current.

1Patent No. US 6,452,165 B1
The Variable Multicollector

Eight moveable collector supports and one fixed center channel are installed on the optical bench of the high precision variable multicollector module. The center channel is equipped with a Faraday cup and optionally an ion counter with or without the retardation lens (RPQ) to achieve the ultimate abundance sensitivity.

The eight detector supports can be precisely positioned along the focal plane, according to the specific needs of the application. The maximum distance between the outermost channels corresponds to a relative mass range of 17% sufficient for the simultaneous measurement of $^4\text{He}$ and $^7\text{Li}$ or $^{202}\text{Hg}$ to $^{238}\text{U}$.

The variable detector supports are driven by motors. Beneath each variable detector platform there is a position sensor located inside the vacuum chamber. Precise in situ monitoring of the detector position directly at the optical bench of the variable multicollector ensures reliable positioning, which is a must for high precision isotope ratio measurements at high mass resolution.

Multiple Ion Counting (MIC)

Each moveable support can carry either a Faraday cup, or a miniature Secondary Electron Multiplier (SEM) or a combination of both in a package. All detectors are of "plug-in" design and can be readily exchanged. It is possible to equip one detector platform with a package of ion counters plus one Faraday cup. The above combination is perfect for counter packages for specific elements in the high mass range e.g. lead and uranium because the packages can be built very compact.

The configuration where the ion counter packages are attached to the outer moveable Faraday cups (H4, L4) keeps the full flexibility of the Faraday cup array. The insertion of the additional ion counters at these outer positions does not block any Faraday cup configuration. A fully equipped system can be loaded with a maximum of 17 channels: 9 Faraday cups plus 8 ion counters - all of which can be used in a simultaneous multicollector measurement.

\[ \text{PATENT NO. US 6,949,732 B2} \]
The Amplifier

Each Faraday cup is connected to a current amplifier. The amplifier signal is digitized by a high linearity voltage to frequency converter with an equivalent digital resolution of 22 bits. This ensures sub-ppm digital resolution of all measured signals independent of the actual signal intensity. The amplifiers are mounted in a doubly shielded, evacuated and thermostated housing with a temperature stability of ± 0.01°C.

The dynamic range of the current amplifiers is extended to 50 V in positive ion detection mode. For negative ions it is restricted to 15 V. The extended dynamic range supports the measurement of large isotope ratios, and it directly leads to an improved signal to noise ratio for the minor isotopes.

For classical systems the need for a precise cross calibration of the current amplifiers defines a precision barrier in static multicollection. Even with perfect Faraday cups giving uniform response, results of static measurements are biased by the accuracy and reproducibility of the gain calibration. In the classical method of cross calibration, a high precision, constant current source is sequentially connected to all amplifiers. However, with this method, amplifiers cannot be calibrated to better than ~5 ppm per channel. For instance if one considers an isotope system consisting of three isotopes the best external precision can be estimated to be: 5 ppm x √3 = ~9 ppm.

The Virtual Amplifier

The goal of the new multicollector development was to break through the 5 ppm precision barrier. The TRITON and the NEPTUNE use a patented measurement procedure, which completely eliminates gain calibration biases: the Virtual Amplifier concept. In all previous multicollector systems the relation (connection) between individual Faraday cups and amplifiers was fixed. In the Virtual Amplifier concept all Faraday cups involved in a certain measurement are sequentially connected to all amplifiers. As a result all signals have been measured with the same set of amplifiers and for the calculation of the isotope ratios all calibration biases of the amplifiers are cancelled.

Key Technologies

- 50 V Dynamic Range
- Elimination of Amplifier Biases
- No Cup Factors
- Up to 17 Ion Beams can be detected simultaneously

*Patent No. US 6,472,659 B1*
**Measuring Large Isotope Ratios**

The measurement of large isotope ratios is affected by scattered ions generated at slits and apertures, the flight tube walls and most importantly the interaction of ions with residual gas particles. Ions which suffered one of these interactions have lost kinetic energy and/or have changed their direction of motion. As a result, these ions appear at incorrect mass positions along the focal plane, typically increasing background at neighbouring masses. The TRITON and the NEPTUNE employ an optional Retarding Potential Quadrupole Lens (RPQ) that acts as a high selectivity filter for ions with disturbed energy or angle.4

With the TRITON, whose thermal ionization source produces ions with a small energy spread (0.5 eV), the RPQ reduces the abundance sensitivity by two orders of magnitude from typical 2 ppm ($^{238}\text{U} \pm 1$ u) to 20 ppb. The dark noise of the ion counting system used in the RPQ is less than 10 counts per minute. This combination of low dark noise and high abundance sensitivity allows the determination of large isotope ratios with the highest accuracy. Combining the RPQ with the NEPTUNE, whose ICP source generates ions with an energy spread up to ~5 eV, improves the abundance sensitivity by one order of magnitude from guaranteed 5 ppm to 500 ppb with more than 90% transmission.

The abundance sensitivity of the NEPTUNE can be further improved by increasing the energy barrier of the RPQ filter: At 50% transmission, an abundance sensitivity of 150 ppb can be achieved. However, the stability of the system will be reduced.

4Patent No. US 5180913

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**Thermo Scientific TRITON: abundance sensitivity with and without RPQ.**

**Thermo Scientific NEPTUNE: abundance sensitivity without RPQ filter.**
Thermo Scientific TRITON

Thermal Ionization Source
The thermal ionization source is characterized by a very small (~0.5 eV) kinetic energy spread of the ions. Therefore, a single focusing geometry that focuses for angular divergence only is fully sufficient. Chromatic aberrations due to the initial energy spread of the ions can be neglected. In this configuration the magnetic sector lens focuses ions of different mass along an inclined focal plane with 45° angle. The magnet is laminated for high speed peak jumping and low hysteresis. The inner width of the flight tube is 14 mm, ensuring minimal scattering. Baffles are present along the flight path to directly catch any diverging ions and to minimize scattering at the side walls.

The New TI Source
The new ion source optics of the TRITON have been optimized for maximum ion transmission for both single and double filament techniques. It makes the TRITON about twice as sensitive as the MAT 262. The new sample turret holds 21 single or double filaments. The filaments can be easily exchanged without using any tools.

Special care has been taken by shaping the ion source lens elements so that the build up of contaminations and memory in the source are minimized. The lens stack is easily accessible by the user for inspection and maintenance.

The ion source is held at an acceleration potential of 10 kV to achieve optimum sensitivity.
The Zoom Optics

Multi-dynamic measurements can be used to eliminate cross calibration biases of Faraday cup detectors or multiple-ion-counting (MIC) detectors. The philosophy of ‘no compromises’ led us also to achieve the ultimate performance using this procedure.

Historically, the collectors had to be set to compromise positions in order to fully catch the ion beams in all different cup configurations. The Zoom Optics is a tool to change mass dispersion. If used synchronously with switching the ion beams, perfect overlap of all peaks in all configurations is achieved. This scheme is fully integrated into the TRITON’s automatic measurement.

For instance, the Zoom Optics allows measurement of all isotopes of UO in the same detector configuration as U without the need of mechanical readjustment of the detector positions.

Multicollector configurations for Nd and Sr, along with the amplifier rotation scheme (Virtual Amplifier)
Thermo Scientific NEPTUNE

Double Focusing High Resolution Multicollector ICP-MS
The kinetic energy distribution of ions generated in an ICP source is large (~20 eV), compared to ions from a thermal ionization source. A double focusing analyzer, focusing both ion energy and angular divergence, is the best technical solution for this challenge.

Reduced Energy Spread Using a CD-System
The NEPTUNE’s ICP interface reduces the initial kinetic energy spread from ~20 to ~5 eV by capacitively decoupling (CD) the plasma from the load coil using a grounded platinum guard electrode. This low kinetic energy distribution, together with a wide energy acceptance of the mass analyzer and 10 kV ion acceleration voltage, eliminates all effects of ion energy spread on isotope ratios and mass bias.

Plasma Interface at Ground Potential
The plasma interface is held at ground potential, allowing easy access to the nebulizer, spray chamber and torch. Changing from solution to laser ablation is as easy as the connection of an autosampler.

The plasma interface can be isolated from the analyzer through an automatic gate valve. The ion transfer optics focus the ions from the plasma interface onto the entrance slit of the double focusing analyzer. Mass bias is mainly generated in the plasma interface and the ion transfer optics. The NEPTUNE’s excellent mass bias stability, sensitivity and low background result from Thermo Fisher Scientific unique ion transfer optics.5

5 Patent No. US 5180913
Interference Free Measurements by High Mass Resolution Multicollection

High Mass Resolution
The ion optics of the NEPTUNE achieve high mass resolving power on all detectors along the image plane. This capability is based on its refined ion optics with

- Almost coincident angular and energy image planes
- Large focal depth due to large ion optical magnification (see page 6)

The NEPTUNE can be operated in three different resolution settings: Low, medium and high resolution. In high resolution settings the resolving power can go up to \( m/\Delta m = 10,000 \). The \( m/\Delta m \) is derived from the peak slope of the rising edge measured at 5% and 95% relative peak height.

For single collector sector field instruments the mass resolution is changed by switching both the source slit width and the detector slit width. For high mass resolution a small source slit and a small detector slit is used. This typically results into very narrow triangular shaped peaks in the mass spectrum and ensures safe peak separation of interfering species. However, for high precision isotope ratio measurements a wide peak flatness range is required and triangular peak shapes cannot be used. In order to separate molecular interferences from elemental peaks on a multicollector instrument a small source slit has to be selected as well, however, the detector slit can be kept at low resolution setting.

The individual detectors of the variable multicollector can be positioned such that just the elemental ions can enter the detector whereas the interfering ions are stopped on one side of the detector slit. The typical operation mode of a multicollector instrument is a static operation mode where the magnetic field remains constant and the interferences are stopped at the detector slit.

According to the systematics of the nuclear mass defect all molecular interferences in the low and medium mass range are heavier than the elemental species and all interferences can readily be stopped at the same side of the detector slit. The use of the wide detector slit for all resolution settings is the best choice because it guarantees the widest peak flatness at high resolving power, which is a must for high precision and accurate isotope...
Software Package

The Thermo Scientific TRITON and NEPTUNE Software Package

Most of the software modules are common to both instruments:
• Cup configuration editor to define and select cup configurations
• Method editor to set up user-defined measurement procedures
• On-line and off-line data evaluation packages including statistical capabilities and display of the results in spreadsheet or graphical form
• Sequence editor for automatic, unattended acquisition and evaluation of samples including sample/standard bracketing and blank subtraction.
• Automated report generation of analytical results.

Tuning the Source

The TRITON (TI source)
• Fully automated sample turret manipulation
• Configurable and automated filament heating
• Pyrometer readout of the filament temperature

The NEPTUNE (ICP source)
• Fully automated plasma start sequence
• Easy auto sampler setup

Method Setup

• Selection of cup configuration
  • Cup position
  • Faraday or SEM
  • Assignment of isotope masses to the detector
• Data collection strategy:
  • Static measurements
  • Dynamic measurements
  • Fast single collector peak jumping measurements
• Integration of sample heating program (TRITON)
• Selection of bias/fractionation corrections
• Definition of isotope ratios
  • Outlier tests
  • Interference correction
  • Equation editor for user-defined data reduction
• Switch key to synchronize start of data acquisition with laser ablation (NEPTUNE)
Sequence Editor

- Automatic acquisition of samples, standards and/or blanks
- Computer control of autosampler
- Online blank subtraction and mass bias correction using an external standard
- Report of delta-values
- Online ASCII export
- Sequence accepts external trigger for starting (i.e. from laser system)

Evaluation

- On-line and off-line evaluation
- User configurable display of results:
  - Spreadsheet
  - Graphical display
- Access to all raw data
- On-line monitoring of ratios, intensities, statistics vs. time

Process Control Language (PCL)

- Script language based on C programming language
- Modification of existing procedures:
  - Baseline determinations
  - Gain calibration
- Definition of new procedures
  - Open for user-defined experiments
- Scripts can be:
  - Run individually
  - Combined with existing software modules

The software runs under the Microsoft Windows® operating system. The software package is optimized for stability, performance and is fully compatible with future operating systems. The software combines the strength of an optimized, Windows-based package written in C++ with the power and flexibility of a user-friendly open structure, realized in our unique Process Control Language, PCL. The Microsoft Windows® operating system allows the data system to be easily connected to a network, enabling data transfer and remote control of the instrument.
Laboratory Solutions Backed by Worldwide Service and Support

Tap our expertise throughout the life of your instrument. Thermo Scientific Services extends its support throughout our worldwide network of highly trained and certified engineers who are experts in laboratory technologies and applications. Put our team of experts to work for you in a range of disciplines – from system installation, training and technical support, to complete asset management and regulatory compliance consulting. Improve your productivity and lower the cost of instrument ownership through our product support services. Maximize uptime while eliminating the uncontrollable cost of unplanned maintenance and repairs. When it’s time to enhance your system, we also offer certified parts and a range of accessories and consumables suited to your application.

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