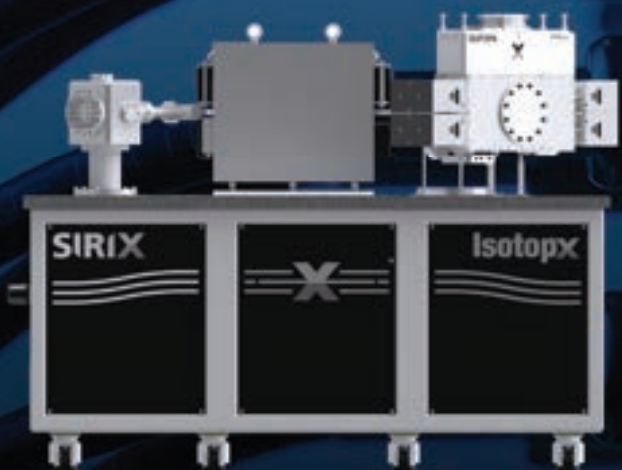


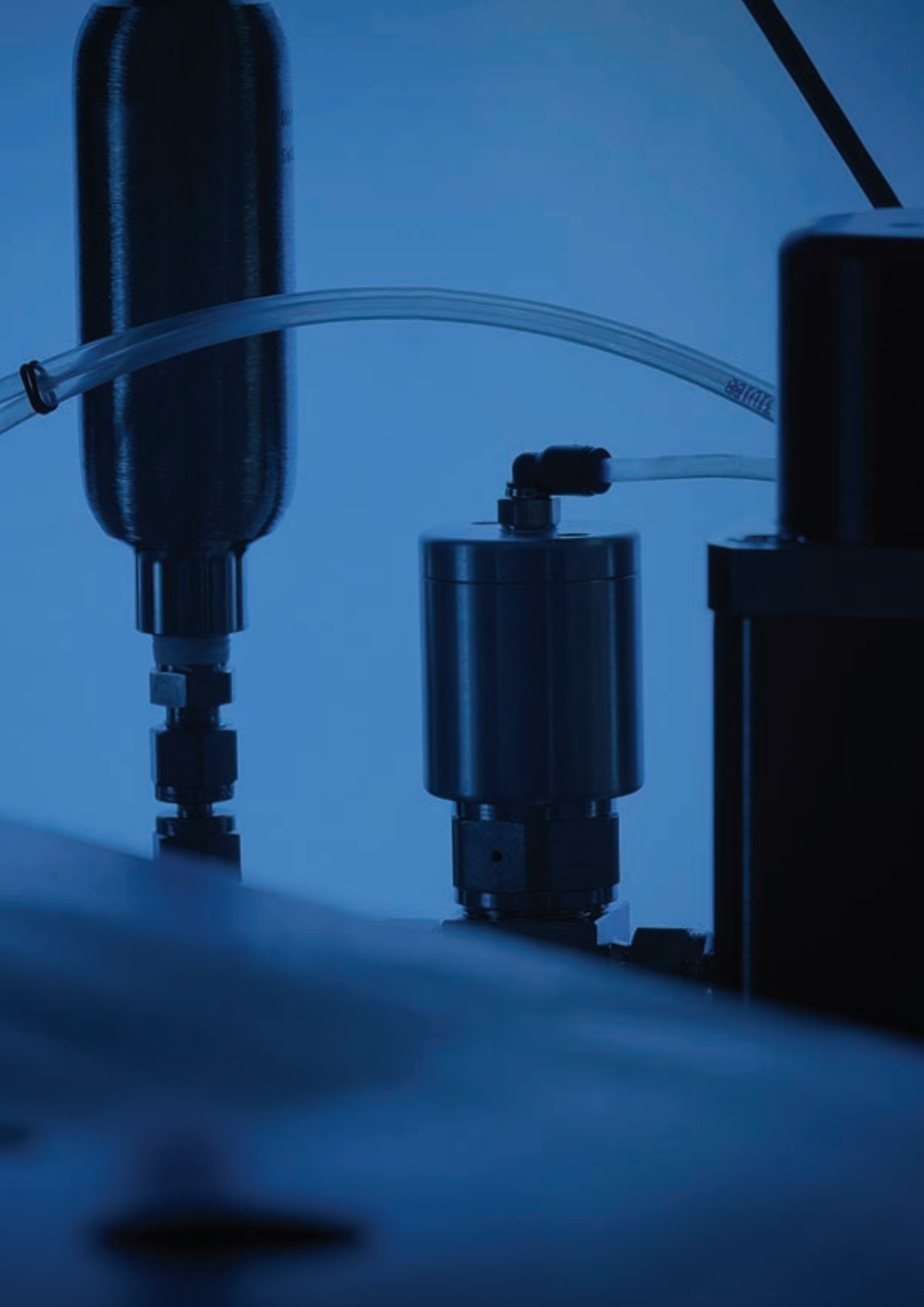
# Isotopx



# SIRIX

Isotope Ratio  
Mass Spectrometer  
with ATONA<sup>®</sup>

Excellence  
in Mass  
Spectrometry



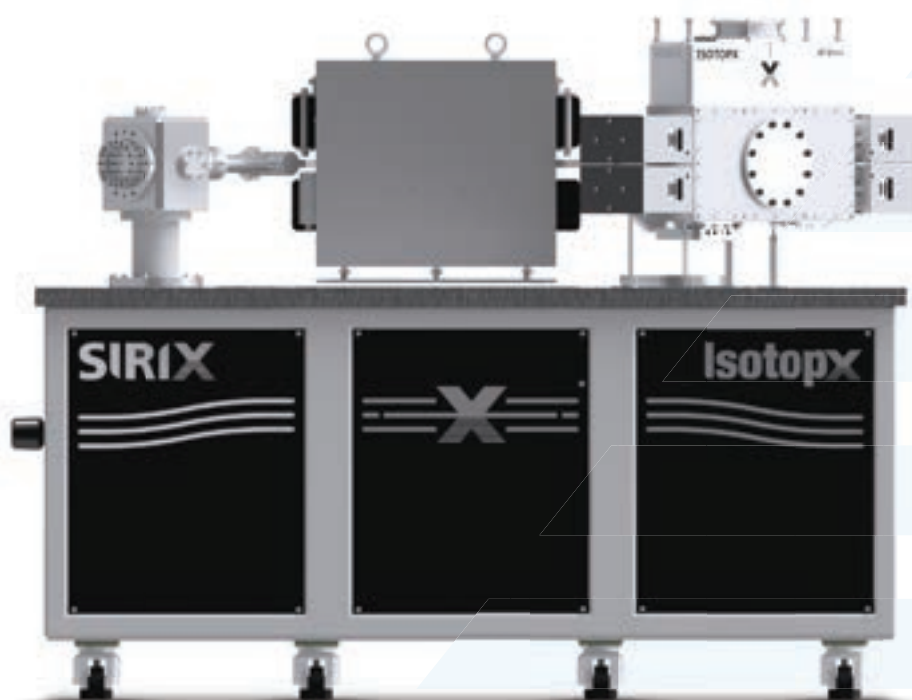
# Why SIRIX?

## *Solving isotope ratio puzzles one step at a time.*

Here at Isotopx we have a proud history in providing isotope ratio solutions. We consider ourselves to be the innovators in the industry, proven by our unique ATONA® and ZEPTONA technologies. By leveraging our technologies and platforms we can offer a wider range of mass spectrometer types – all designed and built with the goal of ultimate precision, ease of operation, and excellent day-to-day reliability.

The SIRIX from Isotopx is a perfect example of this; it's an instrument that benefits from our existing technologies such as TIMS and noble gas MS, yet is designed for a different set of equally demanding isotope ratio applications.

SIRIX is a large radius isotope ratio mass spectrometer (IRMS). It has higher sensitivity and greater resolution than contemporary instruments, all courtesy of our existing ion optics platform. Why do this? Because there are scientific challenges in the world of IRMS where sensitivity and resolution can offer huge benefits, particularly if you are analysing isotopologues or very small carbonate samples. If these are your challenges, SIRIX could be the answer.



# SIRIX

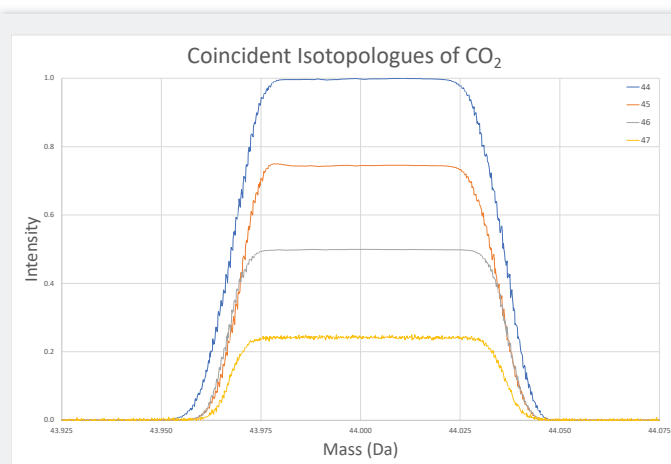
## The new standard in high performance IRMS

**Imagine if... You could achieve better than 10 ppm precision for 48 CO<sub>2</sub> / 44 CO<sub>2</sub>, within 100 minutes.**

In recent years measurement of isotopologues or “clumped isotopes” has become widespread. Focus is on the analysis of CO<sub>2</sub> where isotopes of mass  $m/z$  44, 45, 46, 47, 48 and 49 are of interest. The new SIRIX mass spectrometer from Isotopx features advanced multicollector technology derived from the Phoenix Thermal Ionisation MS. It also includes the ATONA<sup>®</sup> amplifier in combination with a high sensitivity, high mass resolution spectrometer design. The result is a powerful, versatile, sensitive, stable isotope mass spectrometer that is intuitive to use, and can also be optimised for the most exacting applications.

SIRIX includes up to 9 individually movable Faraday collectors, allowing complete flexibility in the choice of isotope analysis. The ion optics are based on the same magnet design as the Phoenix TIMS. A large 90° 27 cm radius magnet provides sufficient mass dispersion to allow for simultaneous multicollection of all CO<sub>2</sub> isotopes. The wide flight tube ensures no backgrounds from ion reflections under the minor isotopes. Interferences from hydrocarbons are eliminated from peak centres due to the high mass resolution (>500, 10% valley). A mass resolving power of 5,000 is obtainable.

The large dynamic range and low noise of the ATONA<sup>®</sup> allows the accurate and precise measurement of ion signals of >1e-7 A down to <1e-17 A on the Faraday array, essential for CO<sub>2</sub> analysis.



### CO<sub>2</sub> Measurement, 6,000 1 s Integrations

Function	Mean (Aft)	Std Dev% (Aft)	Std Err ppm (Aft)	Included	Total
45/44	1.18E-02	0.078	1.06	4599	6000
46/44	4.19E-03	0.072	0.97	5618	6000
47/44	4.68E-05	0.170	2.28	5544	6000
48/44	4.46E-06	0.636	8.58	5508	6000

The M20 multi-collector sets the SIRIX apart. Up to 9 individually motorized Faraday collectors are fitted, all on the same focal plane. The mass spectrum above shows multi collection of CO<sub>2</sub> isotopes at mass 44, 45, 46 and 47. The ability to move collectors allows the use of narrow Faraday collectors. Resolution is increased and the problems associated with wide collectors are eliminated.

The data summary above shows indicative precisions obtained on the measurement of CO<sub>2</sub> isotopes. A ~160 nA beam was analysed for 6,000 1 s integrations. This length of time is comparable to sample on-beam time for clumped isotope analyses.

# SIRIX

## The new standard in high performance IRMS

*Imagine if... You didn't need to sample-standard bracket, effectively doubling your sample throughput.*

Existing instrumentation requires switching between sample and reference gas of the order of every 30 s to continually "calibrate" the instrument. Each switch between sample and reference gas has a corresponding delay/settle period for the beam intensity to stabilise. As a result, the duty cycle of sample gas can be well below 50%, limiting productivity.

With the development of the ATONA® amplifier system and new extended range ATONA®, Isotopx has successfully managed to improve performance and stability of the amplifier system. The exceptionally quiet and stable amplifier allows for extended measurement times of sample gas, without the need for repetitive calibration with a reference gas, or calibration of different gain resistors.

### BETTER PRECISION

# 10 ppm

Achieve better than 10 ppm precision for 48 CO<sub>2</sub> / 44 CO<sub>2</sub>, within 100 minutes

### BETTER STABILITY

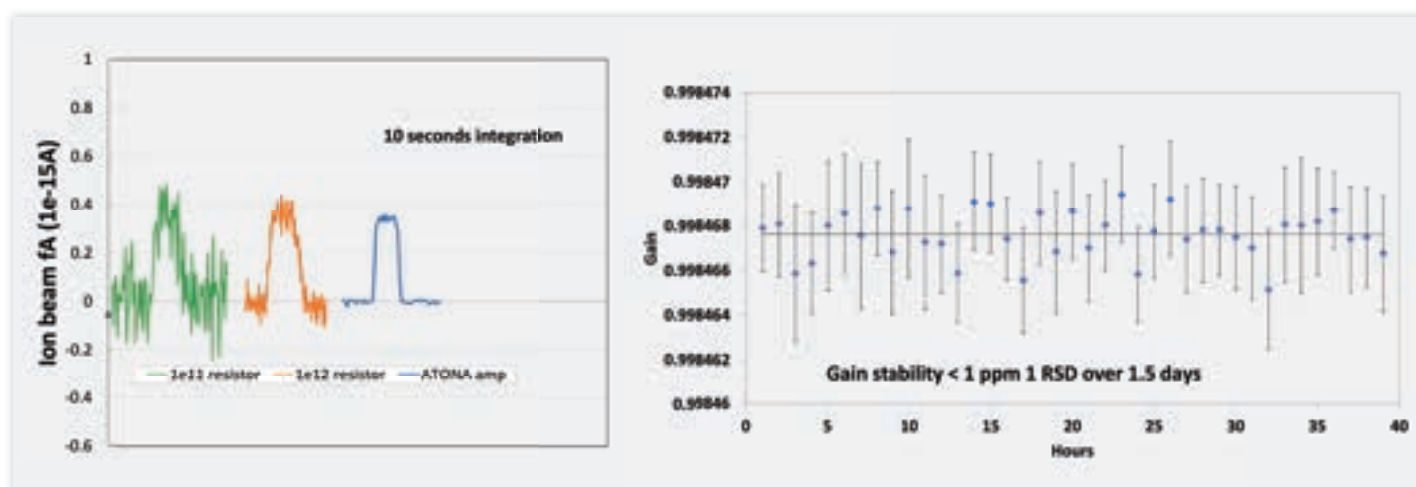
# 1 ppm

ATONA® shows better than 1 ppm stability over a 40 hour period, with extremely low backgrounds too

### INCREASED PRODUCTIVITY



SIRIX reduces your calibration requirements, increasing your sample throughput



Peak shapes of the same sized ion beam scanned using different detector technologies. It can be seen that the ATONA® amplifier peak exhibits much lower noise characteristics than 10e11 or 10e12 resistor amplifier peaks.

Here you can see the gain stability using the ATONA® amplifier, showing better than 1 ppm stability over a 40 hour period. This is not possible using traditional resistive amplifier techniques.

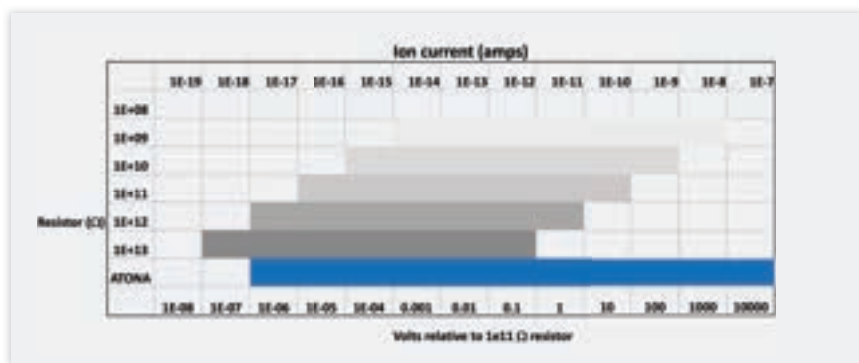
# SIRIX

## The new standard in high performance IRMS

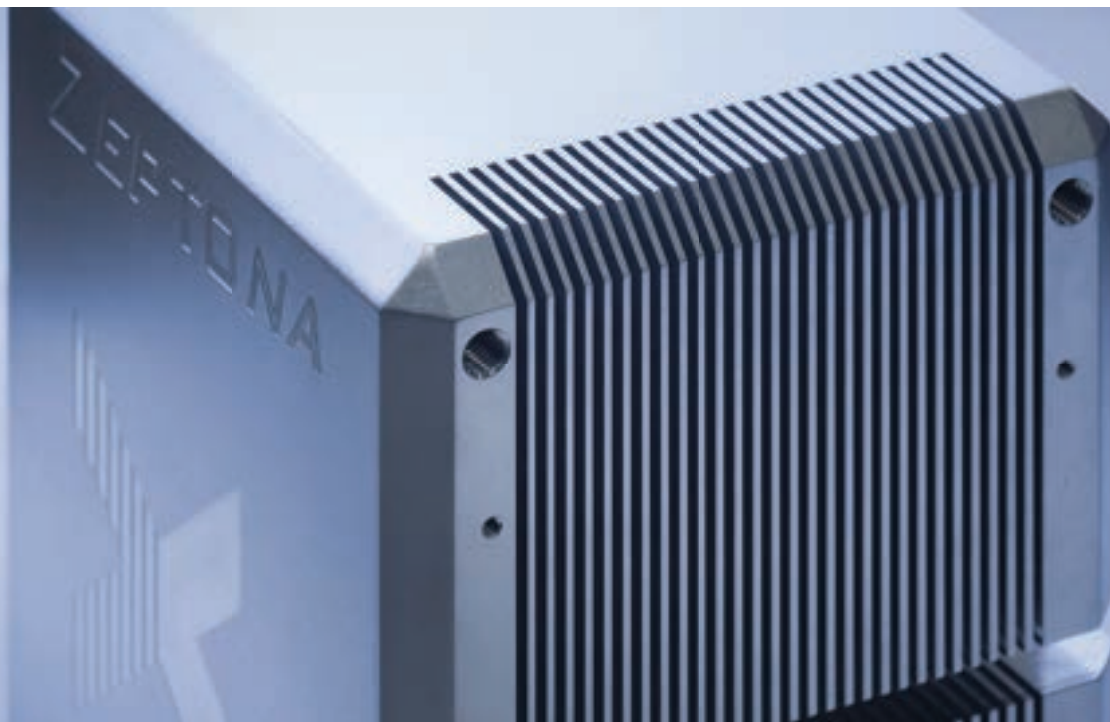
**Imagine if... You didn't need to calibrate your detectors, or choose your resistor according to application or beam size.**

The unique ATONA<sup>®</sup> amplification technology from Isotopx has eliminated the need for a "feedback resistor". The outcome is a significant reduction in amplifier noise, a dramatic increase in dynamic range, rapid amplifier decay, and improved baseline and calibration stability. The new extended range ATONA<sup>®</sup> is fitted as standard and increases maximum signal measurement to 200 nA on channel 1 and 20 nA on channels 2 to 9. This allows the instrument to run with much greater signal intensity. Correspondingly the time taken to achieve the required precision is much shorter, increasing sample throughput. The ATONA<sup>®</sup> amplifier also exhibits extremely stable baseline measurements over extended periods of time.

The dynamic range of the ATONA<sup>®</sup> amplifier is far wider than that of traditional resistive amplifiers. The image below shows a dynamic range comparison of resistive amplifiers and ATONA<sup>®</sup> referenced to a 1e11  $\Omega$  amplifier.



SIRIX has additional optional technologies including a high abundance sensitivity filter, ZEPTONA amplification technology, and an adjustable source slit.

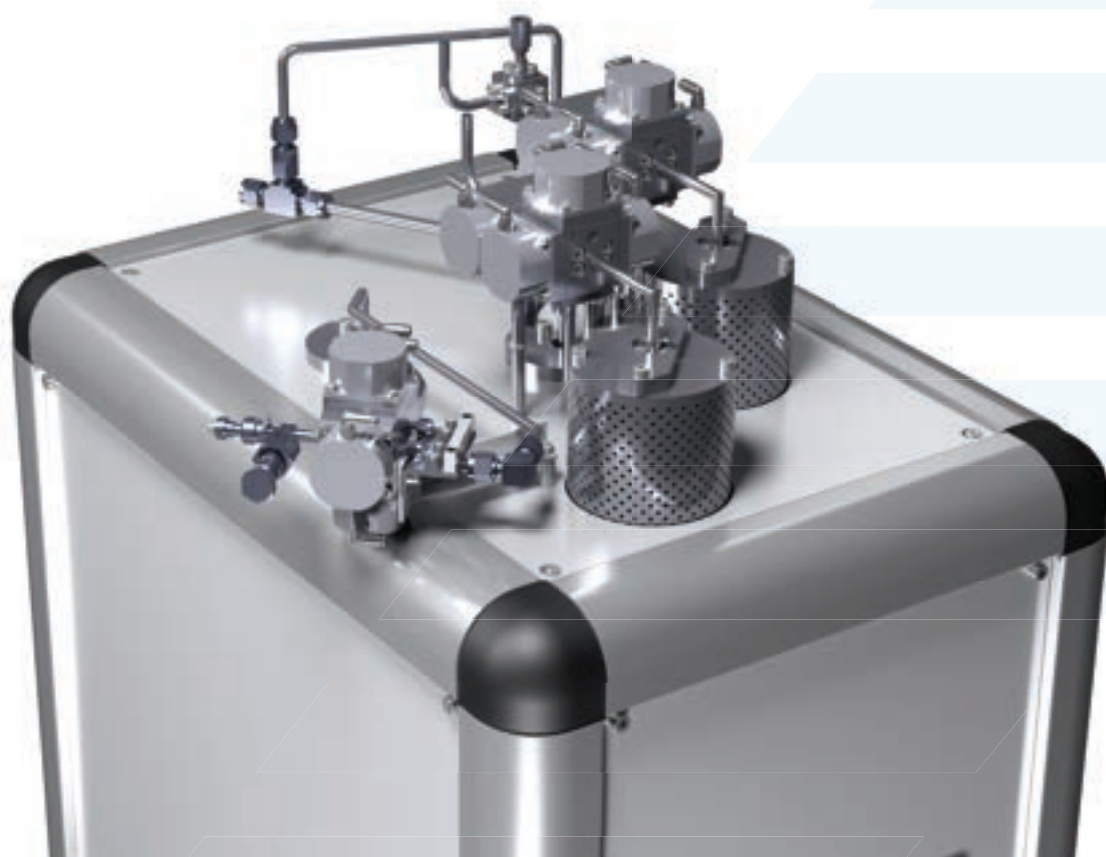


# SIRIX Dual Inlet

Naturally, there are isotope ratio applications where the highest precision and long-term reproducibility are of the utmost importance. Many IRMS users with these requirements choose to use a “dual inlet” device. In simplistic terms this is an automated inlet device that allows a direct comparison between a known standard and unknown samples, to the benefit of measurement precision and accuracy. The technology has been widely used for several decades and is well understood.

The dual inlet from Isotopx combines proven design with today’s workflow techniques and analysis methods. The all-stainless steel construction provides long life operation of the valves which is combined with a dual turbo-pumped vacuum system to maintain sample integrity. Two adjustable gas volumes are provided as standard, traditionally referred to as the sample and reference bellows. These gas volumes have been engineered with exceptionally tight tolerances to guarantee reproducibility. A non-adjustable micro volume, for small samples, is available and attaches directly to the sample valve block. Valves and pipework flow path have been minimised to reduce any dead volume.

Operation of the dual inlet is fully controlled by the SIRIX software. During normal operation, the dual inlet runs in automated mode. The superior performance of the ATONA® detector system is leveraged to allow real-time rebalancing of the bellows and is no longer dependent on the integration period of the analysis. Manual valve operations, vacuum control and dual-inlet status and are controlled through an inlet mimic within the tune window.



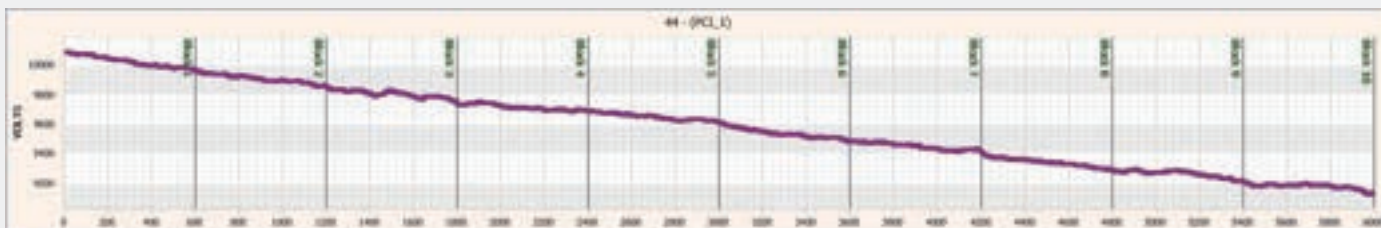
# CO<sub>2</sub> Measurement

*Let's look at the performance of SIRIX for CO<sub>2</sub> in a bit more detail...*

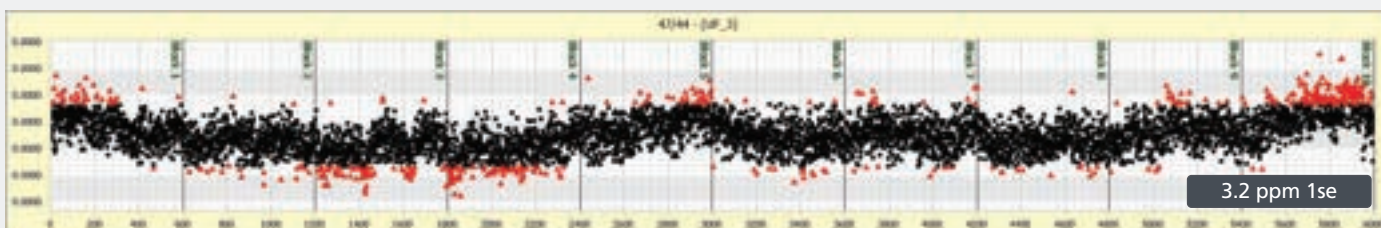
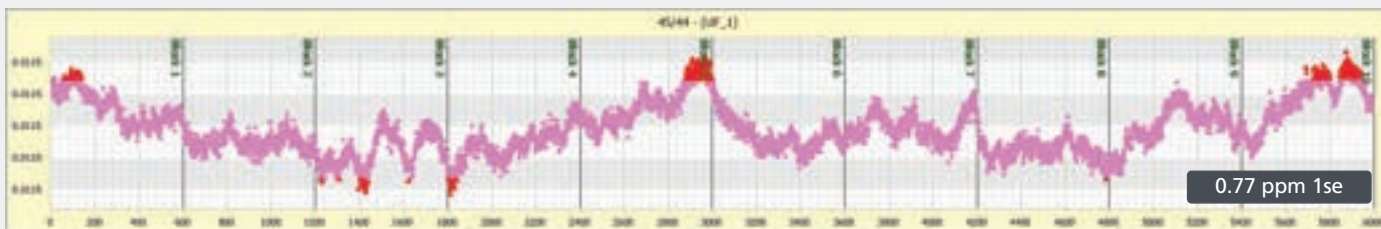
To see how well the SIRIX performs as a mass spectrometer, we've measured a fixed volume CO<sub>2</sub> sample over time, without any form of internal or external correction. Any instabilities related to the instrument would become readily apparent.

The figures below show typical ion beam behaviour over the course of 100 minutes. Each data point is a 1 second integration. A total of 6000 integrations were made, in 10 blocks of 600. The ion beam was peak centered at the start of each block. The ion signal of the 44 CO<sub>2</sub> starts at just over 1000 volts (relative to a 1e11 ohm resistor) or 1e-8 amps. It decays slowly over the period by about 10%, as would be expected. No ion focusing was done during the acquisition.

The correlation between the 54/44 and 47/44 isotope ratios is clear to see, with no drift. The scales are somewhat exaggerated and indeed these "raw" isotope ratios represent a **precision of 0.77 ppm 1se** and **3.2 ppm 1se** respectively.



m/z 44 intensity as a function of time over 100 minutes.



45/44 and 47/44 ratios over the same time period.



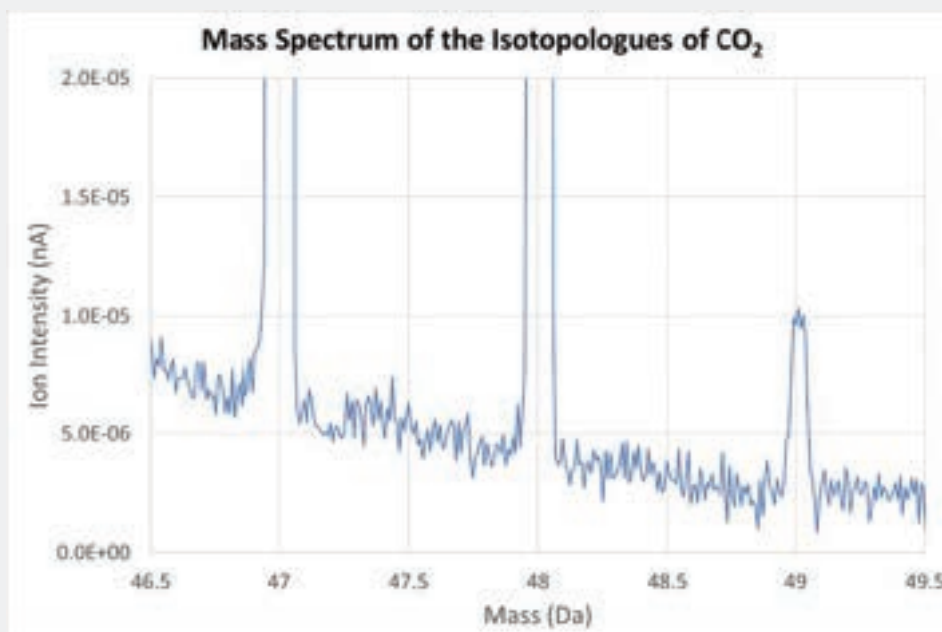
# Baseline Measurement

## What about baselines and the issue with peak tailing?

The importance of accurate baseline measurement is demonstrated in the figure below, which shows the high mass peak tailing from the  $m/z$  44 peak beneath the minor isotopes 47, 48 and 49. The 44 signal is  $1.4 \times 10^{-7}$  amps. The 47 peak is off-scale at  $6.3 \times 10^{-12}$  amps. The peak tail at mass 47 is  $5 \times 10^{-15}$  amps, so without a tail correction the contribution of the peak tail under mass 47 is approximately 0.1%.

At mass 48 the uncorrected peak tail is approximately 1% of the 48 peak. There is no evidence of any other baseline artefacts, for example from collisions with the flight tube. These reflections would produce larger errors in isotope ratios with increased ion intensity and would prevent an improvement in precision with increasing ion intensity. The lack of reflections is due to internal baffling and the wider flight tube than in some contemporary instruments.

The large  $\text{CO}_2$  isotopologues are extremely low abundance. At mass 47, the abundance is 0.07 ppm relative to 44, at mass 48 it is 0.03 ppm, and it is  $<0.01$  ppm at mass 49. Yet all the peaks are clearly resolved from the peak tail. The peak tail at mass 47 can be exactly quantified by measuring  $m/z$  46.5 and 47.5 and taking the average of the two intensities. For mass 48 the baseline is measured at 47.5 and 48.5. For 49 a baseline at 48.5 is used. Baseline subtraction can be made for each integration. This is important because during analysis the ion signal is constantly reducing, and baselines taken at the start of the measurement are not applicable during the measurement.



The high mass peak tail from mass 44 beneath 47, 48 and 49. No electrostatic filters are needed to remove the peak tail as the baseline can be corrected for with each ratio.

# Other Applications

## *Can SIRIX be used for any other applications?*

SIRIX is a large radius IRMS designed specifically for isotopologue measurement and for high precision carbonate measurement. But are there are other applications where SIRIX can offer substantial gains.

For example, the measurement of argon isotope ratios for paleotemperature applications has traditionally been done using static vacuum mass spectrometry due to the limitation of sample size (often sub-picomole size samples). However, this may not produce precision equal to that possible by dual inlet IRMS.

For measurement of these isotope ratios where sample size is more abundant, for example with trapped air bubbles from ice cores, then dual inlet IRMS can produce significantly more precise data, potentially in the tens of ppm 1se range.

With its high sensitivity, massive linear dynamic range, and independently adjustable collectors, SIRIX is an ideal “dynamic” mass spectrometry solution to this analytical requirement.







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