

## SPECIFICATION

### Isotope Ratio Mass Spectrometer for high precision measurement of the relative isotope abundances of $^{13}\text{C}$ , $^{15}\text{N}$ , $^{18}\text{O}$ , $^{34}\text{S}$ and $^2\text{H}$ (D)

#### 1. Scope:

This Specification describes the requirements for an Isotope Ratio Mass Spectrometer (IRMS) (hereinafter referred to as the “System”) for high precision measurement of the relative isotope abundances of  $^{13}\text{C}$ ,  $^{15}\text{N}$ ,  $^{18}\text{O}$ ,  $^{34}\text{S}$  and  $^2\text{H}$  (D)

The System shall be fully compatible with the peripheral modules already present at the laboratory, such as: Universal continuous flow interface, Elemental Analyser and Gas chromatograph (For details please refer to Appendix 1)

The End-User of the System is the Federal Fluminense University, Niterói, Brazil

#### 2. Applicable Documents:

The following documents shall be applicable for this Specification to the extent specified hereinafter:

2.1 CODEX Guidelines on the use of Mass Spectrometry (MS) for Identification, Confirmation and Quantitative Determination of Residues, CAC/GL 56-2005

2.2 ISO/IEC 17025 General requirements for the competence of testing and calibration laboratories.

In the event of conflict between the documents listed above and the content of this Specification, the content of this Specification shall take precedence to the extent of the conflict.

#### 3. Functional and Performance requirements:

The System shall meet the following functional and performance requirements:

3.1 High sensitivity electron impact self-aligning ion source.

3.2 Ion source parameters controlled by a data system.

3.3 All ion source parameters to be set by the data system. The ion source parameters shall be automatically optimized, stored, loaded and appended to specific gas configurations.

3.4 Mass range from 1 to 80 u at full acceleration voltage.

3.5 Resolution better than 110.

3.6 Universal triple collector suitable for all standard applications involving  $\text{N}_2$  and  $\text{CO}$  (28, 29, 30),  $\text{NO}$  (30, 31, 32),  $\text{O}_2$  (32, 33, 34),  $\text{CO}_2$  and  $\text{N}_2\text{O}$  (44, 45, 46), and  $\text{SO}_2$  (64, 66) comprising one narrow and two wide Faraday cups with individual 50V amplifiers for simultaneous analysis of up to three ion beams and additional two faraday cups for  $m/z$  2 and  $m/z$  3 collection in dual inlet and continuous flow mode.

- 3.7 Absolute sensitivity of at least 1200 molecules CO<sub>2</sub> per m/z 44 ion under normal Dual Inlet operating condition.
- 3.8 Sensitivity under continuous flow conditions of at least 1500 CO<sub>2</sub> molecules per m/z 44 with He load will guarantee an isotope ratio linearity better than 0.02 ‰/nA.
- 3.9 System Stability: < 10 ppm on mass scale.
- 3.10 H<sub>3</sub><sup>+</sup> Factor: < 10 ppm/nA.
- 3.11 Read back of system status parameters such as accelerating voltage, emission current, magnet current, turbo molecular pump status and vacuum pressures.
- 3.12 Software package for checking diagnostic functions all-important aspects of the mass spectrometer.
- 3.13 Multiple user licenses for data evaluation.
- 3.14 PC hardware and software:
  - 3.14.1 PC and flatscreen
  - 3.14.2 Colour printer
  - 3.14.3 Data acquisition software for continuous flow measurements and off-line data manipulation
  - 3.14.4 Software shall provide automatic, multi-point isotopic calibration and output sample delta values with respect to internationally accepted reference scales
  - 3.14.5 Software shall permit automatic drift and blank corrections if required. Drift correction shall be possible between definable sample positions within a sequence

#### 4. Marking:

The System shall have all safety markings in English language or Portuguese language.

#### 5. Packing:

For shipment the System shall be packed in accordance with international standards that are applicable for the shipment by air/sea of this kind of equipment.

#### 6. Quality Requirements:

- 6.1 The System shall be manufactured, shipped and installed in accordance with the Supplier' ISO quality assurance system or an equivalent quality assurance system.
- 6.2 The Supplier shall document the compliance with this quality assurance system.

#### 7. Testing and Acceptance:

The System, after installation, shall be tested by the Supplier together with the End-User to demonstrate that the performance meets the manufacturer's performance specifications and the minimum requirements specified herein as determined by the IAEA and the End-User.

The results of the testing of the System shall be documented by the Supplier in an acceptance protocol that shall be signed by the End-User.



8. Installation and Training:

The Supplier shall install the System at the Federal Fluminense University, Niterói, Brazil;

The Supplier shall provide one day training for up to three staff of the End-User in the operation and maintenance of the System at the End-User's location immediately after the installation of the System.

9. Deliverable Data Items:

The Supplier shall provide two complete sets of operation and servicing manuals and technical drawings in the English language.

10. Optional Items:

At the request of IAEA/End-User, the Supplier shall provide the spares parts required for the System, as per Appendix 2.



### **Appendix 1- Modules present at the counterpart Laboratory:**

The Isotope Ratio Mass Spectrometer (IRMS) system shall be able to control and operate with current Interfaces that have been purchased by the laboratory:

- Flash EFCt Elemental Analyser with integrated carrier box for isotope ratio measurement and temperature regulated electronic flow controller, including MAS200R autosampler with 32 position sample drum, Eager software for IRMS computer. Manufactured by Thermo Fisher Scientific;
- GC IsoLink II for C, N and H including TRACE GC 1310 with split/splitless injector with digital pressure and flow control (DPFC 1000 kPa) for the accurate and precise on-line determination of  $^{13}\text{C}/^{12}\text{C}$  and  $^{15}\text{N}/^{14}\text{N}$  isotope ratios in organic mixtures. The GC IsoLink is directly connected to the gas chromatograph. Manufactured by Thermo Fisher Scientific;
- ConFlo IV Universal Interface. It allows the simultaneous attachment of two high flow preparation units like elemental analysers and one low flow unit like GC-C/TC III to the Isotope Ratio MS. The ConFlo IV allows the fully automated and unattended switch between preparation units.5 Reference Gases are constantly attached. All reference gases are available by computer control. Manufactured by Thermo Fisher Scientific.



**Appendix 2- Spares parts required for the IRMS system, ConFlo IV Universal Interface, GC IsoLink II, Flash EFCt Elemental Analyser**

- Spare parts and consumables for GC IsoLink (manufactured by Thermo Fisher Scientific, Reference number 1240201);
- Gas Sampling Valve (6-port) for Trace GC (manufactured by Thermo Fisher Scientific, Reference number 1272730);
- FID detector for TRACE GC ULTRA (monitored in ISODAT) (manufactured by Thermo Fisher Scientific, Reference number 1147891);
- Subambient oven cooling, liqu. N<sub>2</sub> cryogenic system (manufactured by Thermo Fisher Scientific, Reference number 1147950);
- PoraPLOT Q fused silica capillary column 25 m x 0.32 mm (manufactured by Thermo Fisher Scientific, Reference number 0171911).