# **SPECIFICATION FOR**

# THE PROVISION OF ION CHOMATOGRAPHY SYSTEM

**UK SBS PR19096** 



#### **Specification Document – Supplies & Services**

Title of Request:	UK SBS PR19096 ION CHROMATOGRAPHY
Required Delivery Date:	NO LATER THAN 20/03/2020
Required Commissioning Date:	INSTALLATED and COMMISSIONED by NO LATER THAN
	END OF MARCH 2020

#### 1. Introduction

ISIS pulsed neutron and muon source is a world-leading centre for research at the Science & Technology Facilities Council (STFC), Rutherford Appleton Laboratory (RAL) near Oxford, in the UK. Our suite of neutron and muon instruments give unique insights into the properties of materials on the atomic scale.

The ISIS Deuteration Facility supports ISIS Users experiments by providing deuterated compounds for use within beamline experiments. The group is responsible for the synthesis of simple and more often large complex compounds. Part of this, we have a requirement to analyse the samples produced before handing over to the users. The type of samples that we produce range from simple perdeuterated fatty acids to complex surfactants where purity with respect to ion comtent is important. For certain systems the presence of other ions can have a major effect on the outscome of beamline experiments.

Other systems also involve ion exchange, and in order to see whether this exchange has taken place an ion chromatography system is important.

#### 2. Aims & Objectives

- 2.1. We require an Ion Chromatography System that is capable of analysising the ion contents of ionic liquids (eg anion purity, halide impurities), anion or cation counterions in surfactants (eg sodium, lithium, potassium dodecylsulfates, metal ion impurities eg Ca) and potentially analysis of carbohydrates and amino acids.
- 2.2. The Ion Chomatography System must meet the brief and fulfil the minimal requirements set out below.
- 2.3. The Ion Chomatography System would be located within the Deuteration Facility, for the sole use by the Deuteration team.
- 2.4. It is required that the instrument is delivered, installed and commissioned by no later than end of March 2020.

#### 3. Background to the Requirement

- 3.1. The Deuteration Facility has recently undergone a refurbishment and as part of this the size of the facility has been expanded to include an annex for analytical equipment.
- 3.2. The ISIS Deuteration Facility supports ISIS Users experiments by providing deuterated compounds for use within beamline experiments. The group is responsible for the synthesis of simple and more often large complex compounds. Part of this, we have a requirement to analyse the samples produced before handing over to the users. The type of samples that we produce range from simple perdeuterated fatty acids to complex surfactants where purity with respect to ion comtent is important. For certain systems the presence of other ions can have a major effect on the outscome of beamline experiments.

Other systems also involve ion exchange, and in order to see whether this exchange has taken place an ion chromatography system is important. Whether that be metal anion exchange on a surfactant, or a metathesis of a halide to another anion in an ionic liqud. Both cases require us to quantify the level of all ions in the system.

#### 4. Scope

- 4.1. The requirement is for an ion chromatography system that is capable of analysing the ion contents of ionic liquids (eg anion purity, halide impurities), anion or cation counterions in surfactants (eg sodium, lithium, potassium dodecylsulfates, metal ion impurities eg Ca) and potentially analysis of carbohydrates and amino acids.
- 4.2. The ICS will be housed in the Deuteration facility for sole use by the Deuteration team to analyse samples produced for our Users.
- 4.3. We require the ICS to be delivered with all the required equipment as stated below:
  - Dual channel system to ensure samples run in parallel
  - Reagent free system that generates its own eluents to increase the accuracy of the measurements.
  - Gradient pump system
  - Auto sampler temperature controlled, ability to vary sample vial size, capable of partial loop injection
  - High pressure system capable of up to 5000psi/35MPa to improve resolution and increase throughput
  - Interchangeable detector conductivity and electrochemical with the option of adding others eg uv/vis

- 4.4. The Ion Spectrometer System must be delivered by no later than 20/03/2020 and installation and commissioning to be completed by no later than end of March 2020.
- 4.5. The Ion Chomatography System will be managed in house with no additional technical support staff. We therefore require ICS maintenance to take no longer than one hour per week.
- 4.6. Must include at least 2 years warranty, including any preventative maintenance services required.

## 5. Requirement

- 5.1. The Ion Chromatography System must be capable of analysing
  - the ion contents of ionic liquids (eg anion purity, halide impurities),
  - anion or cation counterions in surfactants (eg sodium, lithium, potassium dodecylsulfates, metal ion impurities eg Ca)
  - and potentially analysis of carbohydrates and amino acids.
- 5.2. The system must have:
  - 5.2.1 Dual channel system to ensure samples run in parallel
  - 5.2.2 Reagent free system that generates its own eluents to increase the accuracy of the measurements.
  - 5.2.3 Gradient pump system
  - 5.2.4 Auto sampler temperature controlled, ability to vary sample vial size, capable of partial loop injection
  - 5.2.5 High pressure system capable of up to 5000psi/35MPa to improve resolution and increase throughput
  - 5.2.6 Interchangeable detector conductivity and electrochemical with the option of adding others eg uv/vis

5.3. The system should be adapted and/or expanded at any time with different versions as well as with other upgrade options.

# 5.4. Training

Onsite training to be carried out for a minimum of two superusers within 2 weeks of commissioning the instrument.

Further training can be included along with prices in a separate document in the Pricing Schedule.

# 5.5. Computer(IT)

5.5.1. It is essential that the IT hardware offered to Contracting Authority by the tendering organisation shall incorporate a workstation grade Computer Hardware System capable of achieving Full Operational Functionality of the proposed instrument. The expected specification should meet or exceed the following example as a minimum:

Intel Xeon or AMD Ryzen or equivalent workstation grade processor (minimum 8-core);

AMD FirePro or Nvidia Quadro or equivalent workstation grade graphics card (minimum 4GB DDR5 RAM);

2TB SSD Storage (in RAID configuration if multiple drives);

32GB DDR4 RAM;

30" 3840x2160 (4K) LED-LCD monitor;

1 GBit Ethernet.

- 5.5.2. It is essential that the proposed IT hardware will have sufficient processing speed, system memory & data storage capacity to allow the proposed system to operate at full functionality for a minimum of 2 (two) Years without either data acquisition or data processing being constrained in any way.
- 5.5.3. The proposed system shall be supplied with a comprehensive software package facilitating full operational functionality. It is expected that this software shall, as far as possible, be intuitive to the user for basic operation and therefore not require extensive training to be provided. The software shall come equipped with an extensive help menu explaining the function of all aspects of the software.
- 5.5.4. There must be provision for a minium of 10 licenses for processing of data away from the attached PC and site network.
- 5.5.5. Software updates, both major and minor versions, should be included for free.

### 5.6. Support

- 5.6.1 Must include at least 2 years warranty, including any preventative maintenance services required.
- 5.6.2 To avoid premature obsolescence, replacement and spare parts for components used in the proposed system shall remain available for a minimum period of 2 (two) Years from the date of their last manufacture.
- 5.6.3 The Contracting Authority shall expect that during the Warranty Period, should it be necessary for one, or more, major Components of the proposed System to be repaired away from the Contracting Authority's premises that Appropriate Replacement Equipment and/or a Demo System will be provided on Free Loan to Contracting Authority for the period of repair.

#### 6. Timetable

6.1. Delivery, Installation and Commissioning:

Delivery of the instrument must be made no later than 20/03/2020

Delivery of the instrument will be made to:

Dr Sarah Youngs R55, Cryogenic Extention, 2<sup>nd</sup> Floor, STFC Rutherford Appleton Laboratory Harwell Campus, Didcot, OX11 0QX

- 6.2. Payment terms are defined as follows:
  - 100% upon completion of installation and commissioning
- 6.3. Installation and commissioning plan to be proposed and must be completed within a week from delivery no later than end of March 2020