AGREEMENT No.
(To be quoted on all correspondence)

FUNDING AGREEMENT

between

THE SCIENCE AND TECHNOLOGY FACILITIES COUNCIL

and

CONSIGLIO NAZIONALE DELLE RICERCHE

Concerning collaboration in mutual scientific research at the spallation neutron source ISIS

The Science and Technology Facilities Council (hereinafter referred to as "STFC"), acting through its Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire, OX11 0QX, United Kingdom.

and

Consiglio Nazionale delle Ricerche (hereinafter referred to as "CNR", Piazzale Aldo Moro, I-00185 Roma, Italy

- desiring to ensure greater collaboration between scientists from the United Kingdom and Italy in neutron scattering research and muon spectroscopy, and in particular in the exploitation of ISIS;

- Wishing to build on progress achieved in previous Italian collaborations and

- recognising the benefits which will accrue to the Italian science community from international collaboration in the exploitation of the ISIS facility;

hereby agree as follows:

ARTICLE 1 - DEFINITIONS

In this Agreement, the following terms shall be used in the sense in which they are defined in this Article.

1.1 "RAL" is the STFC's Rutherford Appleton Laboratory sited at Chilton, Oxfordshire, United Kingdom.

1.2 "ISIS" is the spallation neutron source located at RAL, consisting of a high intensity proton accelerator serving a neutron production target station, with a variety of neutron scattering instruments and associated equipment. The accelerator also serves, independently, a muon beam facility.

1.3 "Instruments" are the neutron scattering instruments and associated facilities, and the muon research facilities, collectively referred to as "the Experimental Facilities".

ARTICLE 2 - OBJECTIVE

2.1 The object of the Agreement is to enable scientists from Italy to collaborate with RAL in the ISIS research programme in order to develop mutually beneficial instrumentation and techniques and knowledge associated with the international utilisation of the ISIS target stations.

2.2 Participation in these activities by other Italian and UK research organisations and universities is welcomed and encouraged. Instrumentation of particular interest to the

Italian community is listed in Annex I. The management of joint instrumentation projects will be mutually agreed.

2.3 STFC aims to explore together with the CNR and other international research organisations to develop further instruments at ISIS.

2.4 CNR agrees to contribute to the funding of the ISIS experimental facilities in accordance with Article 6.

2.5 STFC agrees to collaborate with the CNR in order to ensure that the Italian science community has access via a peer review process to the research facilities and to share in the scientific knowledge which will be made freely available.

2.6 ISIS will work with CNR on education, training and outreach activities aimed at broadening the use of ISIS and related facilities.

ARTICLE 3 - USE OF FACILITY

3.1 A description of ISIS and the associated facilities to be made available under the terms of the Agreement is available at http://www.isis.stfc.ac.uk

3.2 CNR is entitled to submit a bid for use of the ISIS facilities for its scientists in the normal manner and subject to the normal peer review process. The contribution made by CNR at Article 6 of this Agreement does not automatically entitle CNR to any rights to access or use the ISIS facilities, or any other scientific research facilities, at RAL.

3.3 Scientists conducting experiments under the terms of the Agreement shall receive the normal support facilities accorded visiting scientists, viz:

a) Routine operation and maintenance of instruments.

b) Use of preparatory laboratories and facilities, and provision of standard sample environment equipment.

c) Use of computing facilities for the collection and concentration of data, and sufficient analysis to ensure the integrity of data.

d) Reasonable use of general RAL services.

3.4 Use of ISIS instruments under the terms of the Agreement shall be restricted to scientists normally eligible for support from CNR.

3.5 STFC guarantees entry to RAL of the scientists visiting ISIS under the terms of this Agreement. However, the scientists will only be able to use the ISIS Facility if they have been successful in obtaining permission for experimental research through the peer review process. During their presence on site they shall be subject to the safety, business and other regulations currently in operation and be under the control of STFC's Chief Executive.

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3.6 Should ISIS fail in whole or in part to perform as required for the implementation of the collaboration, STFC and CNR shall consider together the consequences.

ARTICLE 4 - ALLOCATION OF INSTRUMENT TIME

4.1 CNR shall appoint a spoke person for the Italian programme and a coordinator for the management of the CNR annual contribution towards instruments and instrumentation (Art. 6.3). The CNR Commission for Research at the Neutron and X-ray Facilities shall advise the CNR about the scientific programme and the submission of experiment proposals.

4.2 Applications from Italy shall be assessed scientifically and technically within the framework of the ISIS Facility Access Panels on the same basis as all other applications. Italian scientists shall be included on appropriate selection committees. The costs incurred in attending the selection committees shall be borne by ISIS.

4.3 The experimental schedule shall be drawn up by ISIS, taking into account the Italian experimenters' requirements.

ARTICLE 5 - EXPERIMENTAL RESULTS

5.1 Scientific results arising from experiments carried out under this Agreement shall be freely available and shall be published in accordance with usual academic practice, except where exploitable results arise from an experiment when the procedures of the sponsoring organisation for that experiment (STFC or CNR) shall apply.

5.2 Where experiments are carried out in collaboration with third parties, rights in respect of exploitable results shall be determined by separate agreements between such parties and STFC and CNR.

ARTICLE 6 - CHARGES AND INVOICING

6.1 CNR shall make an annual contribution to STFC as support for ISIS operational costs. This contribution is to be treated as a grant and will be outside the scope of UK VAT.

6.2 The annual contribution referred to in Article 6.1 is fixed at a level of at least 1.7 M€ for the duration of this agreement, but may be increased by agreement after 2014 consistent with Article 10.

6.3 CNR shall make an annual contribution of 0.8 M€ to the development, construction and operation of specific instruments and instrumentation as specified in Annex I. This contribution may be partially in-kind.

6.4 CNR may make an additional in-kind contribution for collaborative work linked to the requirements of the European Spallation Source.

6.5 CNR will pay STFC 50 k€ in every year of the agreement to partially cover travel and subsistence expenses for Italian scientists performing experiments at ISIS under the CNR-STFC Agreement. STFC will administer the above sum on behalf of the CNR, in collaboration with CNR International Relations Office, and shall make an annual report to the this Office on the use of these funds. Funds not used in a particular year will be carried forward to the next year.

6.6 Invoices for the annual costs will be submitted to CNR on 1 April in each year of the Agreement commencing on 1 April 2014. Payments are to be received by STFC within two months of the invoice submission dates.

ARTICLE 7 - INJURY TO PERSONS AND DAMAGE TO PROPERTY

7.1 STFC and CNR undertake not to make one another liable for damage or personal injury or death of any person, except in the case of gross negligence of STFC and CNR or any person for whom STFC or CNR is responsible.

7.2 STFC shall use all reasonable endeavours to safeguard the property of all visitors to RAL under its normal operating and safety arrangements. For their part, staff supported by CNR and other persons at RAL for the CNR's purposes, are responsible for observing security procedures at the site in respect of themselves and their property, including any requirement not to enter restricted areas.

7.3 STFC's responsibilities under the Health and Safety at Work Act 1974 of any statutory modification or re-enactment thereof are not removed or amended in any way by Articles 7.1 and 7.2 above.

ARTICLE 8 - DURATION, TERMINATION AND EXTENSION

8.1 This Agreement is deemed to start on 8 March 2014 and shall continue for six years, unless one of the parties gives notice before 1 March 2015. The agreement shall be reviewed during the calendar year 2019 to consider its extension.

8.2 Either party may terminate this agreement before the end of the period specified in article 8.1 above, with not less than six months notice in writing, if funding for the Agreement is withdrawn or for other reasonable cause.

ARTICLE 9 - OWNERSHIP

9.1 Equipment provided by CNR in association with Article 2.1 shall remain the property of CNR for the duration of the agreement. Thereafter ownership shall pass to STFC as a donation of that equipment for use in scientific experiments of an international nature.

9.2 CNR shall be responsible for all expenses concerned with the importation of equipment and shall meet the cost of any taxes or duties that may be levied whether in Italy or the UK in this connection.

9.3 Documents, information etc. provided by CNR and STFC shall remain the property of the disclosing Party and shall not be disclosed to any third party, except for the purposes of this Agreement, without the consent in writing of the provider, such agreement not to be unreasonably withheld. STFC and CNR shall take all reasonable measures to keep confidential information which is received from the other Party under this Agreement and which is specified by the disclosing Party to be confidential at the time of disclosure or which may come to one Parties knowledge or is disclosed to it as a result of work carried out on each other's premises.

9.4 This undertaking shall not apply to information which either at the time of disclosure or after disclosure is published or is made generally available to the public other than through a breach hereof or information already in the receiving Parties possession at the time of receipt and which was not acquired directly or indirectly from the disclosing Party or information acquired by the receiving Party in good faith from a third Party.

ARTICLE 10 – AMENDMENT TO THE AGREEMENT

10.1 This Agreement may be amended subject to the mutual agreement in writing of both Parties.

ARTICLE 11 - LAW

11.1 The Agreement shall be considered as an Agreement made in England and subject to English law.

ARTICLE 12 - DISPUTES

12.1 All disputes arising between the two Parties concerning the interpretation or application of this Agreement which cannot be resolved by agreement shall be referred to an arbitration tribunal appointed by the International Chamber of Commerce in Paris. STFC and CNR shall bear their own costs and an equal share of the cost of the arbitration proceedings. Arbitration proceedings shall take place in London.

ARTICLE 13 - FURTHER INFORMATION

May be obtained from:

STFC - Rutherford Appleton Laboratory
Sales Contracts, Building R74
Chilton
DIDCOT
Oxfordshire
OX11 0QX
England

STFC

Technical Enquiries:	Prof R McGreevy	Tel:	+44 1235 445599
		E-mail	robert.mcgreevy@stfc.ac.uk
Contractual Enquiries:		Tel:	+44
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CNR

Technical Enquiries:		Tel:	+39 06 49932057
		Fax:	+39
		E-mail	virginia.codanunziante@cnr.it
Contractual Enquiries:		Tel:	
		Fax:	
		E-mail	

For and On behalf of CNR

Signed _____ Date - 6 FEB. 2014

Name: Luigi Nicolais Position: President CNR

For and on behalf of STFC

Signed _____ Date 4/3/14

Name: Prof R McGreevy Position: Director ISIS, STFC

Signed _____ Date _____

Name _____ Position: _____

ANNEX I

Instruments and instrumentation development

Below is a list of potential areas for collaborative development of instruments and instrumentation.

Target Station 1

A) INES operation

INES is the experimental station operated under the scientific leadership of CNR. CNR will allocate 100 k€ per annum to STFC for the salary of the INES instrument scientist and to maintain and operate the INES beamline at ISIS. ISIS will hold this money on behalf of CNR acting as paymaster in respect of the costs to be met on CNR's behalf.

A) TOSCA upgrade.

The TOSCA spectrometer at ISIS was funded by the CNR to replace its predecessor TFXA. TOSCA remains to this day the highest-resolution inelastic neutron spectrometer in the world over an unrivalled energy-transfer range (25-4000 cm^{-1}). As such, it represents a superb example of the unique capabilities afforded by short-pulse spallation techniques, e.g., tight (chemical) resolution over a broad spectral range.

An upgrade of the TOSCA spectrometer on ISIS-TS1 will be transformational for the chemical sciences. Detailed neutronic simulations as part of on-going collaborative efforts between ISIS and CNR team have established that use of present neutron-guide technology in the primary instrument will deliver a 1-2 order-of-magnitude increase in detected flux on this instrument. This new capability will be transformational, enabling the chemistry community to tackle materials-chemistry challenges of direct relevance to societal needs and long-term economic sustainability. These include: gas sequestration by nanoporous media e.g., uptake of flue and greenhouse gases like carbon and sulphur dioxide by metallo-organic frameworks; the rational design of graphene-based nanostructures and nanocomposites for next-generation carbon-based functional materials and sensors; chemical catalysis of industrial relevance, including the synthesis of biomolecules like vitamin A using Lindlar-type catalysts or iron-based Fischer-Tropsch catalysts for the efficient liquefaction of coal to make synthetic fuels; new charge-storage and fuel-cell materials relying on the transport properties of light atoms such as hydrogen or lithium at intermediate temperatures; and a plethora of advanced materials such as negative-thermal-expansion materials or thermoelectrics.

B) Improved Engineering Diffraction Instrument.

ENGIN-X is a world class dedicated engineering instrument. There are primarily two types of experiments carried out on ENGIN-X - residual stress measurement and in-situ experiments to observe micromechanical properties of material. The success of ENGIN-X is based on : (*i*) continually development to make the use of instrument more user friendly (*ii*) offering a wide range of sample environment equipment (*iii*) a dedicated and expanding user community especially in the area of industrially applied research. At present the oversubscription is a factor of approximately five, with a significant demand from industry enabled through a new access scheme pioneered at ISIS. This level of oversubscription is now detrimental to the academic and industrial user community. To

satisfy both the capacity and capability demands requires a new instrument to complement ENGIN-X.

A new facility (preliminary name ENGIN-XXX) with the capability for residual stress measurement will serve the growing user community. The specification for the new instrument has similar (or better) resolution to ENGIN-X combined with increased flux. The resolution of the current ENGIN-X meets the present demand for residual stress measurements. However for approximately 10% of the in-situ loading experiments there would be significant benefit from improved resolution. The new instrument would provide enhanced capabilities to measure thicker samples (an important capability for real world engineering), improved 2D/3D mapping, and enhanced time resolution for in-situ experiments.

Together with ENGIN-X and IMAT (operational 2015) the new instrument would provide ISIS with a unique suite of capability and capacity to address the increasing challenge of materials engineering.

C) New interdisciplinary instrument developments on INES

Neutrons have the capability of penetrating several centimetres of material, and therefore are particularly suitable for the study of thick artefacts (e.g. metal objects, marbles, pottery, etc.), or thick processed food (e.g. contaminants for food safety assessment) that cannot be studied with other techniques (e.g. X-rays). Areas of application of non-destructive integrated neutron and optical methods include radiation issues on artefacts, transport in security, dating of biological specimens for biodiversity conservation and bio-geography, fraud stalking in food science. These applications are underpinned by the development of the associated hardware and software, data analysis protocols, and new optical-detection schemes. Areas of science and technologies envisaged include:

a) The integrated system for imaging of materials/artefacts making use of particle (neutron) and light probes. We will take advantage of the unique penetration properties of neutrons combined with the different penetration of electromagnetic radiation, to build a tomographic image of the samples under study. The neutron component will be at first a specific development of the INES beamline and subsequently for IMAT beamline. The light component and related detection systems will be based on optical-radiocarbon-dating methods, i.e. optical $^{14}C^{16}O_2$ detection for on-site dating. It is intended to develop a prototype of a new apparatus for optical detection of $^{14}C^{16}O_2$, based on saturated-absorption cavity ring-down (SCAR) spectroscopy, much more compact, easier and cheaper than the one already developed for laboratory use [Galli et al., Phys. Rev. Lett. **107**, 270802] at the Institute CNR-INO in Florence. The implementation of a transportable version will be developed to operate on site at ISIS for the analysis of archaeological objects, for the dating of cultural heritage samples. In particular, the 4.5-μm laser source will be simplified, moving from the intra-cavity difference-frequency generation referenced to an optical frequency comb in the near IR to a system based on 2 quantum cascade lasers directly emitting in the mid IR. One of them will be frequency locked and spectrally narrowed to a molecular line, while the other one will be scanned across the target $^{14}C^{16}O_2$ line. The cooling system relying on dry ice at 195 K will be replaced by a cryogen-free Stirling refrigerator, capable of cooling the spectroscopic cell down to 170 K, thus further suppressing other molecular lines interfering with the target one. The volume

of the sample gas cell will be reduced from about 8 L down to 0.7 L and, correspondingly, the carbon mass required for the measurement from about 70 mg down to 6 mg. The overall size of the opto-mechanical setup (including cryo-cooling) will be about 120x100x70 cm^3 volume and about 100 kg weight. The laser current/temperature drivers, the locking electronics, the data acquisition/processing electronics and the vacuum pump will be hosted in a 19" rack mount with about 180 cm height and about 100 kg weight. The sample preparation, cleaning and combustion will be the same as for accelerator mass spectrometry (AMS), performed by a commercial elemental analyser (EA), but with no need for graphitization of the obtained CO_2 sample. The overall cost of the new setup for $^{14}C^{16}O_2$ concentration measurements will be reduced from about 300 kEuro to less than 100 kEuro (not including the EA). We expect to improve the present sensitivity of 2 pMC (percent modern carbon), approaching the 0.3 pMC achieved by state-of-the-art AMS. This equipment is intended to operate in-situ at the ISIS beamlines for analysis and dating of archaeological samples. It will be installed on INES then on IMAT.

b) The knowledge of the elemental composition of samples is a valuable information in archaeology, providing insights into the production process and the provenance of archaeological artefacts. A research program in this area will be built on the instrumentation and methods developed within the Ancient Charm project [E. Perelli Cippo et al, Nucl. Instrum. and Methods in Phys. Res. A623 (2010) 693–698]. The work program will combine non-destructive techniques based on neutron sources, namely neutron resonance transmission and prompt gamma-ray activation analysis, to enhance the identification of specific elements and isotopes in artefacts. Both resonance energy patterns and neutron capture gamma-ray energies will be used to enhance isotopic identification and pinpoint the position of the elements in archaeological artefacts and in living and processed biological material. Neutron techniques also allow identification/detection of rare elements (lanthanides or rare earths) that can be at the basis of a next generation of traceability strategies for major agricultural commodities, food and any other biological material of plant origin, including wood. Rare earth spectra, when properly investigated may in fact reveal specific features in the biological matrix, allowing exact identification of geographical provenances. This is of special importance for niche productions with high added value [Bentil et al., J. Braz. Chem. Soc. **22**, 2011, Cobb, Analytical Chemistry **39**, 1967, Cullers et al., Chemical Geology **70**, 1988]. To take advantage of the full incident beam area, INES will be upgraded with a 2D position-sensitive neutron detector previously developed for the Ancient Charm European project. Further enhancements to INES include the installation of a high-resolution germanium gamma-ray detector to monitor the energy and time of gamma-rays following neutron capture. The detector will also be available for gamma-ray background studies in different beamlines and beamline ports at ISIS.

D) Optical and neutron integrated methods for excited states neutron spectroscopy

Neutron probing of the excited states of molecular systems can provide a direct access to the quantum states of reactive and highly mobile groups such as O-H in water, that initiate the proton transfer reactions, as well as the modification of the interatomic van der Waals potentials in the light-excited states in noble gases. Feasibility tests will be made in order to develop the methodology and techniques for simultaneous laser excitation and pump-probe measurements, and neutron scattering measurements of

atomic and molecular systems in the excited states, giving access to a description of the quantum states involved. This activity requires the development of dedicated techniques and set –up such as:

- transportable laser instrumentation for the operation at the ISIS neutron beam lines for simultaneous neutron-laser measurements
- dedicated neutron sample containers with optical windows
- integrated pulsed neutron/pulsed laser acquisition systems

Target Station 2

E) Commissioning and exploitation of CHIPIR.

CHIPIR is the first beamline at ISIS designed for chip irradiation with fast neutrons. It will come into operation in 2014. The commissioning of the new beamline will be performed in two stages before and after the beryllium reflector replacement. New detectors for fast neutron spectrometry will be deployed. The instrumentation in support of chip monitoring during irradiation will be commissioned and made more user friendly in the first few years of operation of the beamline.

F) Commissioning and exploitation of IMAT.

IMAT is the first beamline at ISIS optimised for energy selective imaging. It will come into operation in 2015. The IMAT imaging system features energy selective imaging. The latter requires further development which can be addressed during IMAT commissioning and in the first years of operation of the beamline. Improved resolution detectors will be used as they become available. The diffraction detector banks will be completed.