HERCULES
CALL 2015
Medium-sized Research Infrastructure

APPLICATION FORM

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Promoter-spokesperson for the application (only one allowed)

Last name  Terryn

First name  Herman

Institution  Vrije Universiteit Brussel

Institution refers to the university, university college, strategic research centre or institution of post-initial education from which the application is submitted.

Requested infrastructure

Title or name of the requested infrastructure

Infra-red Analyses from Macro to Nano Scales
From Novel Self-healing Materials to Jurassic Dinosaur Bone Cells

Summary of the funding (in EUR)

The total amount of the requested subsidisations and the amount of co-financing by the institution(s) and/or the contribution(s) by third party/ies will be filled in automatically once the tables in chapter 3. Financing are filled in.

Funding requested from the Hercules Foundation  942,015,30 €

Total amount of co-financing and / or contribution by third parties

Total subsidisable costs  942,015,30 €

I. Scientific section

1. Information on the requested infrastructure/equipment

1.1. Description of the scientific context of the requested equipment / infrastructure

The text is limited to max 11250 characters, blanks incl.

Five departments (from three faculties Faculty of Science and Bio-engineering Sciences, Faculty of
Recently, several departments (SKAR, AMGC & SURF) initiated the development of an analytical multi-disciplinary and interfaculty platform (Hercules 2013) through the acquisition of a complementary set of X-Ray based equipment. It has enabled many inter-disciplinary projects ranging from documenting the chemical composition of Antarctic micrometeorites all the way to that of the “Manneken Pis”, which even attracted attention of the BBC! A new dynamic has arisen between the teams as illustrated by the Archaeology, Conservation, Palaeontology Interdisciplinary Group (ArCPIG) recently created by PhD’s and Post-docs uniting palaeontologists, archaeologists and chemical engineers around material analyses, launching its first seminar series this September and taking part in the VUB ‘Herfstkamp’ in November 2015.

This proposal takes this analytical venture one step further and leverages the multi-disciplinary research and its unique character within the VUB. This Hercules application aims to acquire new infrared instruments (Fourier Transform Infrared Spectroscope - FTIR + microscope & Nano-infrared instrument) to characterize the functional groups (e.g. carboxylic acid, amine, amide groups) present at the surface of a wide range of materials from the macro to the nano scales and to study mass transfers in nanoporous materials. While FTIR microscope hosts samples up to 10 cm$^3$, NanoIR offers the possibility to retrieve IR absorption spectra from surfaces up to 5 cm$^2$ with a lateral resolution of 30 nm. It is a direct respond to the research needs of the initial three departments, joined in this growing multi-disciplinary and interfaculty platform by CHIS & FYSC. All five groups directly benefit from the to be acquired IR and the already existing X-Ray facilities (Figure 1).

In short, the major advantages of the requested IR facilities are:

- Non-/minimal-destructive analyses
- Larger range of materials (i.e. non-conductive) to be analysed at that scale
- Scale continuum: macro to nano and in atmospheric conditions (no vacuum needed)
- Complementary to X-Ray in analytical targets (e.g. organics, functional groups, etc.)
- Transient analyses under variable environments

The paragraphs below highlight some of the proposed usage by the members of the consortium.

The necessity for state of the art IR spectroscopy facilities stems from the need to stay at the cutting edge of research in a variety of areas. In material synthesis and surface characterization, the analysis of organic adsorbates on metals (oxides), so called hybrid structures, and non-conducting novel materials is of fundamental importance for describing phenomena such as heterogeneous catalysis, electrochemistry, biosensing, molecular electronics, organic photovoltaics, and the characterization of 2D materials. Indeed, the surface chemistry of materials is of crucial importance for understanding material interaction with its surroundings, its functionality and durability. Going from macro to nano scales is of particular interest as most surface phenomena occur in this scale range. Furthermore, nanometre scale differences in chemical nature play an integral role in understanding the underlying mechanisms and properties of the processes and materials listed above. As such, the corrosion protection properties of organic coatings on metals is
largely determined by surface interactions in (humid) atmospheric conditions, the efficiency of catalysts are
dominated by outer surface reactions at the catalyst, and nanoscale phase segregation, and interactions at
the electrode surfaces determine the efficiency of organic photovoltaic cells.

Moreover, in geology, palaeontology and archaeology, it is crucial to apply non-destructive analytical
techniques as the studied specimens are often precious and destructive sampling is not an option. Recent
trends in archaeological science prove that complimentary techniques are required for the holistic
investigation of objects. The combined macro to nano scale IR and XRF techniques constitutes a robust
strategy to investigate an array of objects. This IR approach sheds light on, for example, fossilized dinosaur
bone cell structure and their preservation, illustrating the complex fossilization processes of unmineralized
biological structures. In meteorites, access to IR instruments reveals the distribution and nature of organic
matter, mineral components, such as phosphates, and the presence of water in the mineral structure, even
in nominally anhydrous phases, indicating for example the level of thermal and aqueous metamorphism
that their original parent-bodies underwent. FTIR is optimal to quantify water in glassy ejecta produced
during impact cratering on rocky planets, one AMGC specialities. In addition, IR analysis of meteorites and
terrestrial impact rocks provide contribute to the calibration of planetary rover instruments.

Figure 2 shows an extensive series of (sub)surface analytical tools exists, ranging from vacuum to non-
vacuum techniques, covering a range from macro to nano scales. These methods present drawbacks for the
proposed research projects. For example, X-ray Photo-electron (XPS) and Auger Electron Spectroscopy (AES)
are commonly used to unravel the real chemistry of surfaces. However, they require conducting surfaces, while most systems encountered by SURF consist of hybrid systems, combining an
organic and anorganic component that reduces their conductivity. This issue also profoundly affects groups
performing analysis on non-metallic substrates, such as the research on phase separations in polymer
science (FYSC) and on the outer chemical nature of catalysts (CHIS). Furthermore, the techniques need a
vacuum environment: the electrons that are expelled from the systems cannot reach the detector whilst
other atoms/molecules are present in the environment. Criticism remains whether high vacuum conditions
represent the real systems, encountered in practice. In such conditions, it is impossible to identify the
influence of atmospheric conditions (e.g. moisture, gases) on the probed systems. This is of great
importance for the study of coating failure and self-healing mechanisms of hybrid structures (SURF) as well
as for the study of the interaction of different molecules in liquid/gas phase with novel catalysts (CHIS). IR
spectroscopy techniques solve these issues. IR spectroscopy directly provides molecular structure
information through probing and analysing molecular vibrations in a sample. An IR beam is used to excite
the molecular polarised bond, and the absorbed energy leads to identification of the chemical species.

In the case of precious archaeological and palaeontological samples (Iguanodons bones from Bernissart,
cremated bone from Bronze Age Belgian urnfields, etc.) an interest lies in the detection of organic matter and
the assessment of post-burial alteration in a non-destructive way. Raman spectroscopy, due to its laser
beam excitation method, alters the organic matter permanently. XRF only precisely quantifies chemical
elements heavier than sodium, and does not provide information about the organic content or the presence
of functional groups (OH, CO₃, PO₄), or the internal structure of bones and teeth. Again, IR spectroscopy
techniques constitute the best option. Furthermore, a spectrometer enhanced with far-IR (FIR) investigates apatite (Ca₅(PO₄)₃OH) and distinguish calcitic and aragonitic materials (CaCO₃) in regions of the
spectrum rarely examined.

Additionally, modern IR devices are now equipped with mapping and imaging capacities (at μm scale)
documenting precisely the distribution of various organic components and their association with mineral
phases. Such instruments analyse larger samples (up to 10 cm² under the microscope objective) without
the slightest alteration. In meteorites, such mapping capability documents organic component distributions
at micro and nano scales within different types of carbonaceous chondrites (the most pristine and organic
rich meteorites) and allows comparison with micrometeorites and interplanetary dust particles. Additionally,
the non-destructive capacity of IR is ideal to study the small and rare dust particles obtained by NASA, ESA
and JAXA sample return missions (i.e. Genesis, Stardust, Hayabusa). Studies on terrestrial samples with
similar composition and affected by water alteration provide a more accurate identification of the mineral
species on Mars and help constraining its water history. Finally, to study catalysts (CHIS), the IR
microscope an additional heated stage (up to 600ºC) offers the possibility to investigate samples within
controlled environment conditions. It can also be used to study mineral weathering, and/or crystal and
organic matter behavior under changing temperatures.

The macro to nano scale range represents a particularly important asset. For SURF, the macro and micro scales instruments study interactions occurring on interesting surface features, such as grain boundaries, while the nanoIR offers the possibility to investigate nanoscale chemical nature of coatings and delamination mechanisms, self-healing issues, etc. When looking at meteorites, archaeological and palaeontological organismal remains (AMGC -SKAR), combining microscopy FTIR and nanoIR opens novel research possibilities. Even though destructive analyses are required for nanoIR, it is possible to select the perfect subsample using a large FTIR map, hence drastically limiting the damage (micro-drilling) done to the precious specimen.

The acquisition of a macro to nano IR platform is fully complementary to the existing X-Ray platform, leading to a unique analytical combination of instrument where both elemental composition and organic/functional groups can be determined and quantified in a large variety of materials, in a non- or minimal-destructive way. This allows the VUB groups to remain at the forefront of research in non-destructive analyses of palaeontological and archaeological materials, be a leader in self-healing material characterisation, and become a renowned facility for novel catalysts. Finally, a fully complementary X-Ray-IR, Macro to Nano platform is scarcely available worldwide, and has no equivalent in the Benelux. The VUB research partners strengthen their position at international level through gaining full access to a complementary and versatile analytical arsenal.
Figure 1: Multi-disciplinary Platform

SKAR
Cultural heritage studies

x-Rays
Palaeo-environmental and material provenance research
Surface characterisation

Infrared
Semi-non-destructive analytical platform

AMGC
Geochemistry, Palaeontology & Palaeoclimates

SURF
Electrochemical & Surface Engineering

CHIS
Chemical Engineering & Industrial Chemistry

FISCA
Physical Chemistry & Polymer Science

Industrial and natural zeolites
Structured materials
Coating development
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Medium-Scale Research Infrastructure - with a minimum value of EUR 150,000 and a maximum of EUR 1,000,000 including the non-refundable portion of the VAT
1.2. Description of the requested infrastructure

Description of the infrastructure/equipment (including description of the upgrades to be provided), max. 1000 characters, blanks incl.:

**MACRO/MICRO - Vertex 70v + Hyperion 3000, Bruker**
The Vertex 70v is a FTIR spectrometer which can operate under vacuum (if needed). It covers mid- and far-infrared (6000 to 50 cm\(^{-1}\)) with a spectral resolution down to 0.16 cm\(^{-1}\). Combined with an ATR (Attenuate Total Reflectance) unit, it analyses powdered samples and films. The Hyperion 3000 (microscope attached to Vertex) enables the creation of 2D-maps (lateral resolution up to 2 \(\mu\)m and 2D-imaging with a 64*64 pixels detector) in a non-destructive way. The microscope can handle samples as large as 10 cm\(^3\).

**NANO - The NanoIR2, Anasys Instruments**
The NanoIR2 delivers with a 30 nm lateral resolution, infrared absorption spectra. The equipment consists of a pulsed laser with a repetition rate of 1kHz, tuning range of 900-3600 cm\(^{-1}\) and a special resolution of 6 cm\(^{-1}\). The AFM has a scan range of 80 \(\mu\)m *80 \(\mu\)m. An anti-vibration table is included in the quote, being necessary for a good working of the equipment.

Description of the housing (including specific installation requirements, conversions, new construction, etc.) and phasing of the construction works (max. 1000 characters, blanks incl.):
Both instruments are to be installed on the VUB campus Etterbeek. The macro/micro-scale Vertex FTIR & Hyperion microscope will join the \(\mu\)XRF set up within the Analytical, Environmental and Geo-Chemistry unit (AMGC). An air conditioning system will soon be installed in this room to ensure optimal working conditions. No other special construction works are needed for the installation. The NanoIR2 will be located within the research group Electrochemical and Surface Engineering (SURF). The instruments will be fully accessible to all partners, according to the same proven procedure (training, reservation, data processing) currently used for the X-ray instruments.

Description of the permits required (e.g. planning permission, environmental permit, etc.), max. 1000 characters, blanks incl.:
No permits are required, as the requested instruments do not necessitate adjustments to the existing building infrastructure. To our knowledge, no special environmental permits are required for this infrastructure. Future users will be made fully aware of potential risks whilst working with the equipment and will need to take adequate safety precautions.
1.3 Does it involve the acquisition of new infrastructure/equipment or the expansion/replacement of existing infrastructure/equipment? (only one possibility)

- acquisition of new infrastructure/equipment
- replacement of existing infrastructure/equipment
- expansion of existing infrastructure/equipment

Explanation and justification (max. 1000 characters, blanks incl.):
This completely new infrastructure fully complements the newly acquired X-Ray facilities allowing, when necessary, the non-destructive analyses of samples gathering information about major and trace elements together with data on the organic content and structure of the samples.

What infrastructure/equipment do you already have at your disposal (max. 1000 characters, blanks incl.)?

SURF
- FE-SEM-EDX-WDX
- SEM-EDX
- FE AES
- XPS
- TOF-SIMS-cluster ions beam -AFM system
- μ-Raman spectroscopy
- 3 spectroscopic ellipsometers (in situ, visual & infrared)
- TIS
- 2 AFM
- SVET
- SIET
- SECM

AMGC
- 4 gas IRMS
- cavity ring-down spectroscopy
- HR-ICP-MS
- microsampler (<50μm) video & computer driven
- Access to 2 MC-ICP-MS and 1 Solid Source TIMS at ULB via BIGE
- μXRF + Tracer portable XRF

CHIS
- 2 devices for batch adsorption experiments
- 5 systems for reaction and separation experiments
- PSA
-N₂ & Hg porosimetry
-2 high pressure/temperature gravimetric devices, high pressure volumetric setups
-2 vapor gravimetric devices
-8 GC(-MS)
-2 MS
-9 HPLC
-Micro-Milling Robot
-100-node computer cluster
-3 Fluorescence CCD microscopes
-Ar Laser (6W)

**FYSC**
-8 DSC, 2 microcalorimeters, 2 chip nanocalorimeter, 2 TGA, 1 DMA, 2 DR
-FTIR + UV-Vis
-GPC
-2 AFM + 1 Nano-TA
-PALS

**SKAR**
-total station
-GPS receiver & handheld controller
-magnetometer

If it is an expansion and/or replacement of existing infrastructure/equipment, specify the year of purchase of the existing equipment/the year of installation of the existing infrastructure, the financing body, etc. (max. 1000 characters, blanks incl.):

Not applicable

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1.4 Similar equipment/infrastructure

State the similar equipment/infrastructure known to you in your own institution(s) and/or in Flanders. Explain the need to have this equipment/this infrastructure yourself to carry out the research work if the equipment/infrastructure is already available in your own institution(s) or in Flanders. (Maximum 3750 characters, blanks incl.)

**FTIR + Microscope**
Classic FTIR is an established method with a wide range of applications used for the detection of organic matter and the study of molecular interactions. It is present in several Flemish institutions. The combination of infrared spectroscopy and microscopy also exists for decades but its performances have drastically increased over the last few years with the current possibility to map large samples and very high resolution (2 μm). As such, several Flemish universities have recently acquired one or more infrared instruments with microscopy (Hyperion 2000 at UGent, UHasselt & KULeuven - see list below). We opted for the Hyperion 3000 (so far not available in any Flemish universities) that allows much faster mapping through imaging using focal plane array detectors (FPA). Compared to mapping that measures one by one the infrared spectra of several points of the samples, imaging allows measuring the infrared spectra (4,500-900 cm⁻¹) of
a whole section (340*340 μm) in one single measurement. This allows much faster acquisition of data and the analyses over time of a particular area. Combined with a unique stage that can be heated up to 600°C within controlled environment conditions, it allows the study of various material properties, including the uptake rate of guest molecules by the nanoporous materials, and the follow up of the dynamics of self-healing and delamination processes of organic coatings in hybrid structures. The choice of a Vertex 70v resides in its ability to acquire a full range spectra from mid to far-IR in one single measurement compared to the 80v. We will acquire two microscope objectives (Si and Ge). The Si objective is necessary to investigate the far infrared zone, however it is less performing between 1500 and 600 cm⁻¹ than the Ge objective, which does not extend below 600 cm⁻¹, hence the need for both objectives. Finally, the macro instruments available at other Flemish institutions are all heavily used. The utilisation of IR instruments by all 5 groups implies an almost constant usage, which on its own fully justifying the absolute need to acquire such instrument at the VUB.

Modern FTIR microscope instruments in Flanders
-Vertex 70 + Hyperion 2000 (UHasselt)
-IFS 66v + IRscope II infrared microscope (UGent)
-Tensor 27 + Hyperion 2000 (UGent)
-Vertex 80v + Hyperion 2000 (UGent & KULeuven)

NanoIR
Based on the set-up offered by Anasys, only one comparable equipment is available in Belgium. This is located in Machelen, Exxon and is not available for third party users. No other instrument is available in the Benelux. In Europe, only Universities in Paris, Rome, Krakau and Manchester possess such facility. As such, the opportunity to purchase such equipment in a well-defined research context at Vrije Universiteit Brussel will leverage tremendously the group’s scientific output. This instrument is very new (2013) and many innovative applications remains to be discovered. Another type of nanoscale IR spectroscopy does exist (Bruker’s Inspire), however this type of equipment does only offer indirect information on the molecular information of the samples and does not provide real IR absorption spectra.

The unique aspect of this proposal resides in the combination of the two instruments, offering the capability to study the very same material in a continuum of scales (macro to nano), and providing non-destructive (or minimal-destructive) analyses. The FTIR microscope induces absolutely no damage to the sample and both the Vertex and NanoIR work only with a minute fraction of material, as for example micro-drilled in an out of sight part of an exceptional museum piece.

Add an image (click on the field and browse to the image)

1.5 Usage plan

Give a plan for the first three years after purchase of the equipment/infrastructure or, if after it has come into service, if it considers a construction, including a statement of the conditions under which any surplus usage time will be made available (against reasonable compensation) to other research groups within and outside your own institution(s) and any third parties. (Maximum 11250 characters, blanks incl.)

The two instruments will be used by all 5 groups with SURF taking care of the training and maintenance of the NanoIR while AMGC will do the same for the FTIR + microscope. The two groups will be the main
users of the respective instruments. The 5 groups agree that on average ~ 5 to 8 days per month will be reserved for the other partners. However as currently experienced with the X-ray platform, flexibility and priorities is the norm. The first two years, the consortium partners will be using the equipment heavily: training staff, developing/testing analytical procedure, and initiating new (joint) projects, involving this innovative platform. If specific opportunities arise, adjustments could be made to accommodate new internal or external users.

Letter of interest are given in attachment both from industry and academia for this novel instrumental set up. Therefore, roughly one year after instalment, a workshop will be organised together with the interested external parties, to stimulate more common projects and promote inter-disciplinary PhD theses. The consortium expects that after two year of instalment of the equipment, the infrastructure can be open for external/commercial use for a maximum of two days a month. We are convinced that Third Party Services using this platform will attract a lot of interest, because of the uniqueness of the equipment and the availability of expertise of scholars from five different, complementary departments.

Maintenance and bookings will be organised by specific persons of the departments (Tom Hauffman, Christophe Snoeck) and all reservations will be stored in an online management system. A detailed plan of usage by the different groups and their respective and joint projects are shown in Figure 3.
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<table>
<thead>
<tr>
<th>Project</th>
<th>Description</th>
<th>Budget (EUR)</th>
<th>Duration (months)</th>
<th>Type</th>
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<td>48</td>
<td>Innovation</td>
</tr>
</tbody>
</table>

### HERC Bureau - Brussels

**Add an image (click on the field and browse to the image)**
If several institutions are involved in the application, you must draw up a management plan for the equipment/infrastructure.
If third parties are involved in the application, the management plan must expressly state when and how they can exercise the right to use the equipment/infrastructure.
If users other than those given in 1.4. and 1.5. are involved, you must add the list of users here (surname and first name, institution, research group, address, telephone number, e-mail)

**not applicable**

**Estimated usage time** (only two characters allowed)

85  % usage time for own research groups of the consortium

5   % usage time for other research groups within the institutions of the consortium

5   % usage time for external research groups

5   % usage time for third parties (e.g. companies)

100 % total amount of estimated usage time

1.6 **Location of the requested infrastructure**

- in your own research group (local)

- in a pooled facility; name facility below:

  Campus Etterbeek, laboratories on 8th floor in building F + 5th floor in building G

Give a short motivation for your choice of the location of the requested infrastructure. (Maximum 1000 characters, blanks incl.)
The nanoIR will be placed in the research department SURF. This department can be recognised as one of the most important research groups concerning surface analysis worldwide. The other partners in the research consortium already have very extended collaborations using the in house equipment of SURF (see publication list). Likewise, for the FTIR + microscope, the most appropriate location is next to the μXRF hosted at AMGC, who also enjoys a long experience in the management and maintenance of large-scale infrastructure such as mass spectrometers.
2. Qualifications of the research groups concerned

2.1 Scientific added value of the requested equipment/infrastructure for the research of the partners concerned

Give a description of the scientific added value of the requested equipment/infrastructure for the research of the partners concerned. (Text limited to maximum 4000 characters, blanks incl.).

**SURF**

Using the novel IR platform, SURF will be able to analyse on the nanoscale, hybrid structures in true atmospheric conditions. As such, it becomes possible to follow the influence of atmospheric influences on protective organic coatings and look in situ at the self-healing mechanism of materials. Very importantly, the local analysis of the chemical nature of materials will be combined with the electrochemical analysis of systems, e.g. by impedance spectroscopy. This capacity does not exist yet within the analysis scope of SURF, nor of many research groups within the European context. The combined microscope - FTIR equipment of the platform also looks at μm scale phenomena (such as events happening on grain boundaries) and offers the opportunity to study much bigger samples (e.g. parts of Manneken Pis) in non-destructive way.

**AMGC**

FTIR is the perfect tool to characterize organic, carbonate and phosphate contents in palaeontological bones and teeth. For example, the nanoIR can be used to document the complex iron chelation chemistry of dinosaur bone cells to preserve fragments of DNA and proteins. The precise nature of the preservation mechanism still has to be unravelled. In speleothems, these instruments can discriminate between calcite and aragonite fabrics and recognize organic matter serving as a proxy for important climate parameters (i.e. Tº & vegetation activity). In meteorite and impact crater material, IR analyses can provide information on deformation and shock stage of minerals and document the intensity of the collision conditions they underwent.

**CHIS**

The CHIS research includes measuring adsorption equilibria and mass transport on porous materials. In a recent collaboration with the prestigious group of Prof. Kärger (Leipzig) it was shown that micro-imaging techniques, such as the IR-microscopy (IRM) method, can reveal much more information than conventional techniques (paper submitted to Nature Materials). The direct observation of the spatio-temporal accumulation of molecules into single crystals, using the focal plane array (FPA) detector, enables to study the effect of various material properties, including the surface, on their uptake performance. The combination of nano-IR and IRM will allow simultaneously studying transport properties of crystals and analyzing their properties, shedding a new light on the poorly understood surface barrier phenomenon.

**FYSC**

FTIR uses thermal analysis to characterize polymer-based materials from bulk to nanoscale. Often these materials have a micro- or nanoscale structure. Local FTIR studies will bring complementary and crucial information regarding the chemical composition of the phases. As such, the nano-IR perfectly complements our nano-TA AFM-accessory, which is used to study thermal transitions of 100-nm phases, providing a direct link between the local composition and the local thermal behaviour. In OPV research, e.g. knowing the phase compositions in the (nano)phase separated polymer-fullerene active layers will give insight into the formation mechanism of the nanoscale structure and its deterioration upon ageing, which causes the efficiency to drop.

**SKAR**

In addition to the study of archaeological bone and teeth, FTIR has proven to be an effective method in
combination with soil micromorphology as the features identified visually in thin section can subsequently be studied using FTIR to characterise their mineralogical composition or by mapping inclusions' carbonate and phosphate content. Conversely, FTIR permits a fast overview of the compositions of large sediment samples and guide the choice of samples for micromorphological and phytolith analyses. The added value of FTIR includes the identification and characterisation of burnt or charred materials and help distinguish between different types of ashes and fuels contributing to a better understanding of sites' taphonomy by taking into account the preservation state of bone and plant tissue.

Add an image (click on the field and browse to the image)

Provide an overview of the research projects (ongoing, applied for, or planned) that will make use of the equipment/infrastructure. (Text limited to maximum 4000 characters, blanks incl.).

The research projects that will benefit from the acquisition of infrared instruments are detailed in Figure 3 and summarized in the list below. Several of these projects are joint between the different groups such as the ongoing SKAR-AMGC-SURF Hercules 2013: X-ray analytical instrumentation: From the Field to the micro-scale with K. Nys, Ph. Claeys, I. Vandendael, H. Terryn, D. Tys.

**Ongoing projects that will benefit from new infrastructure**

(see table 3 for summary):

- Joint funding SKAR-AMGC-SURF Hercules 2013: X-ray analytical instrumentation: From the Field to the micro-scale - K. Nys, Ph. Claeys, I. Vandendael, H. Terryn, D. Tys

**SURF**
- 1 VUB - OZR & 3 IWT/SIM research projects
- 4 PhDs (Methusalem, Industry, Innoviris, IWT) & 2 Post-docs (FWO, Innoviris)

**AMGC**
- 4 BELSPO (Brains + IUAP), 1 VUB Strategic Research, 3 FWO & 1 AHRC (Arts and Humanities Research Council UK) research projects
- 2 PhDs (FWO & IWT) and 3 Post-docs (FWO)

**CHIS**
- 1 VUB - OZR & 1 FWO Research projects

**FYSC**
- 1 PhD (IWT)
- 1 FWO / European project & 3 IWT/ SIM SBO research projects

**SKAR**
- 3 PhDs (FWO) & 1 Post-doc (FWO)

**Applied for:**

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As shown by Figure 3, there is a lot of demand for IR instruments. A scientific committee, consisting of the promotors of the project, will decide on the user schedule according to research priority, synergy between groups, amount of time required on the instrument, and potential for original developments. The recent experience with the X-Ray facility demonstrates that with a good organisation, the facility can easily accommodate a large amount of projects. Moreover, some users have already used IR instruments at other institutions (i.e. C. Snoeck - Oxford; J. Cousin-Saint-Remi - Leipzig; T. Hauffman - Leuven; etc.), which will speed up the training procedure and allow a direct start of the various projects.

2.2 Strategic added value of the requested equipment/infrastructure

Strategic added value of the requested equipment/infrastructure for the research groups concerned, for the institutions concerned and for the Flemish research area in general. Add also information on the valorisation opportunities (if applicable). Text limited to max. 4000 characters, blanks incl.

As whole, and because of its philosophy of enabling analyses of the very same material in a scale continuum, the requested research platform is unique in the Benelux and scarcely available in Europe. This is especially true if considered in parallel with the X-ray platform acquired in 2014. The infrastructure makes it possible to analyse chemical interactions at interfaces, which at this moment cannot be probed at the VUB. As a result, the partners strengthen their worldwide-recognised expertise in chemical characterisation.

The originality of this project lies in two crucial aspects:

1) The requested infrastructure opens up the possibility to investigate a whole new range of materials in atmospheric conditions on a high lateral resolution surface sensitive level. This is not possible with the now available analysis equipment at VUB. Furthermore, the requested analysis platform with its scale continuum is quite unique in the Benelux. Only one company in Belgium (Exxon, Machelen) owns a Nano-IR, which is not available for external use. Further on, there is, to our knowledge, no such instrument available in the Benelux.

2) The possibility to carry out non-destructive analyses in parallel, both by X-Ray (μXRF) and infrared spectroscopy makes possible the complete characterization of the chemical composition and structure of the material (be it bone and teeth, speleothems, meteorites, historical artefacts, church windows, religious specimens, catalysts, etc.). Adding far infrared capability to the Vertex 70v opens a rarely studied area of the infrared spectra. Preliminary work showed that calcite and aragonite present different peaks in far infrared allowing their differentiation, and preliminary results carried out in the Bruker facilities showed that bone has several absorption bands in that area too that have, to our knowledge, not been investigated. This is perhaps a unique opportunity to better understand the structure of bone composed at 70% of a poorly crystalline inorganic mineral fraction called bio-apatite. Furthermore, only very few studies have
been carried out on modern bone material using NanoIR but, as far as we are aware, none on archaeological and palaeontological remains, once again, giving the VUB the opportunity to become a leader in the infrared study of biological remains and their transformation with time. All this research can, of course, be extended to all other apatitic structures and more. We are not aware that Nano-IR has so far been applied in meteorite research, where it most likely provides complementary information to that commonly obtained by TEM, especially in terms of shock metamorphism generated during planetary collisions. The latter requiring tedious preparation and remains extremely limited in terms of investigated surface, a downside eliminated by the here proposed combination of micro and nano IR instruments. Innovative applications and results are therefore expected.

Therefore, the requested infrastructure creates opportunities for (inter)national collaborations. Furthermore, through the partners in this consortium there is a direct link with other academia. As such, professor Herman Terryn fulfills a part time position at the university of Delft. Through this analysis platform, there will be an increase in common research through PhD and projects.

2.3 Best effort to set-up a consortium and provide co-funding

Describe in no more than 2000 characters, blanks incl., why the application is or is not submitted by a consortium and/or in collaboration with third parties. Describe the actions undertaken to set up a consortium (including third parties). If no co-funding by the institutes or by third parties is available, give the motivations for this decision.

All partners in the consortium are associated with Vrije Universiteit Brussel. However, through the links of professor Herman Terryn the infrastructure will be directly involved in research programs at Technical University Delft (see also letter of support & more than 80 joint publications). This opens up the requested analysis platform to even an international users consortium.

AMGC is also partner with the G-Time Laboratory of the ULB (forming together “BIGE” - Brussels Institute for Geochemical Techniques in Earth Sciences) sharing facilities and often carrying out research in common (see https://we.vub.ac.be/~dglg/Web/Claeys/html/selected_publications_philippe_claeys.html). It is expected that all BIGE staff will benefit from the new IR facility (see letter of support).
2.4 Curricula Vitae of the promoter-spokesperson and the co-promoter(s)

Add an annex for the promoter-spokesperson and for (each of) the co-promoter(s) with:

- A short scientific CV of the promoter-spokesperson and of (each of) the co-promoter(s)
- Academic titles and qualifications

You can add your FWO profile (CV with publications) if you have a FWO account. If not, add (in pdf form) a concise - max. 10 p. A4 per person - scientific CV of the promoter-spokesperson and of (each of) the co-promoter(s), divided into at least the following categories:

- Research output
  - The 10 most relevant publications demonstrating either the relevance of the equipment application or the scientific excellence of the applicants
  - If relevant for the partner(s): (co-)promotership of defended doctorates and those in preparation over the last 5 years
  - Research financing obtained in the last 5 years: (co-)promotership of research projects (with a statement of: the financing body, project title, budget, period)

- Experience of conducting research with and the management of medium-sized research infrastructure, possibly in a consortium or an international context

- Contribution to value-development activities (patents, licences, spin-off creation, etc)

- If relevant for the application or the partner(s): other applicable information
II. Administrative and financial section

1. Information on the promoter-spokesperson

<table>
<thead>
<tr>
<th>Promoter-spokesperson of the application (only 1 allowed)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Surname</strong></td>
</tr>
<tr>
<td><strong>First name</strong></td>
</tr>
<tr>
<td><strong>Institution</strong></td>
</tr>
<tr>
<td><strong>Research Group</strong></td>
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<td><strong>Street &amp; Nr.</strong></td>
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<td><strong>Postal Code</strong></td>
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<td><strong>Date</strong></td>
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<tr>
<td><strong>Signature</strong></td>
</tr>
</tbody>
</table>


Promoter-spokesperson is given emeritus status/retires within 3 years of the project being granted

2. General information

2.1 Nature of application

- Application without partner institution or third party

- Application with partner institution(s) and/or third party (parties)
  
  Please specify below. More than one situation is possible.
  
  - [ ] With partner institutions from within the association (intra-association application)
  
  - [ ] With partner institutions from another association (inter-association application)
  
  - [ ] With third parties

Give the name and address of the receiving institution

Vrije Universiteit Brussel
Pleinlaan 2
1050 - Brussel

Justification for the collaboration

Justification for the intra-association or inter-association collaboration and/or the collaboration with other partner institution(s) (Flemish university/college of higher education) and/or third party (parties): (justification why/why not collaboration with other partners inside/outside the association) (Maximum 3750 characters, blanks incl.)

The VUB consortium (SURF, AMGC, CHIS, FYSC, SKAR) intends to use the IR analytical instrumentation for 85% of the usage time, leaving 5% usage time for other research groups within the VUB, 5% for external research groups and 5% for third parties (e.g. companies). Consequently, VUB research groups will utilise the IR analytical instrumentation for 90% of the usage time, which justifies that no partnership outside the VUB was sought to collaborate in the present application for research infrastructure.
Are you still looking to extend the collaboration to a (an additional) Flemish university and/or university college/college of higher education and/or (a) third party (parties)?

☐ No
☐ Yes

Describe what steps have already been taken to expand the collaboration and what type of body (university, college of higher education and/or third party) or expertise you are seeking. (Maximum 1000 characters, blanks incl.)

not applicable

2.2 Possible ethical and/or biosafety implications

Does the research program with the proposed research infrastructure include (tick if applicable):

☐ Experiments on humans?
☐ Experiments on animal vertebrates?
☐ The processing of personal data (privacy legislation)?

Has a positive ethical advice already been issued?

☐ yes (a copy of this advice must be added as an appendix to the original application)
☐ ethical advice applied for
☐ ethical advice not yet applied for
☐ not applicable
Will you be working with:

- [ ] genetically modified organisms?
- [ ] Biological agents, phytopathogens and/or zoopathogens?

Has the biosafety dossier already been certified?

- [ ] not applicable
- [ ] certification applied for
- [ ] yes, with
  
  ________________________________________________
  
  Biosafety Dossier Code
  
  ________________________________________________
  
  Activity Number
  

2.3. Possible confidentiality implications

Is this infrastructure application part of a project with a confidentiality clause?

- [ ] No
- [ ] Yes entirely
- [ ] Yes partly

Please list below the chapters of this form that come under a confidentiality clause, as well as a brief justification confidential chapters:

not applicable

If yes, a Non-Disclosure Agreement will be signed by the panel members and referees involved in the evaluation and selection.
2.4. Scientific communication

Describe in no more than 1200 characters, blanks incl. what the requested infrastructure is and why it is being purchased in the first place. Give also an outline about the research project in max. 1200 characters blanks incl. in English and an outline in max. 1200 characters blanks incl. in Dutch. If the application is approved, this information may be entirely or partially used for scientific communication (press release or publications for the broader public).

**English version**

In the last years, it has become increasingly clear that chemical information from the outer layers of all objects encountered determine largely their performance and durability. Furthermore, it has been shown from paleontological and archaeological point of view that a lot of valuable information lays in the surfaces which are exposed to the atmosphere. However, until now, the characterisation of this broad range of materials was very difficult as most techniques used are very destructive. The platform FTIR/microscope and NanoIR offers the opportunity to characterise a wide range of materials, providing chemical information from the microscale to the nanoscale. The requested infrastructure combination is unique in the Benelux. It will leverage the individual research outcome of the different partners in the consortium, but also common projects and will put the research of the Vrije Universiteit Brussel again upfront on an international level.

---

**Dutch version**

De laatste jaren is het meer en meer duidelijk geworden dat de oppervlaktechemie van quasi alle gebruiksvoorwerpen en structuren grotendeels hun performantie en duurzaamheid bepaalt. Daarenboven is vanuit paleontologisch en archeologisch standpunt gebleken dat veel waardevolle informatie te vinden is in oppervlakken die aan de atmosfeer werden blootgesteld. De karakterisatie van een breed gamma aan materialen was echter tot op heden erg moeilijk, door het destructieve karakter van de gebruikte technieken. Het FTIR/microscopy en NanoIR platform geeft ons de mogelijkheid om deze materialen chemisch te karakteriseren, met een laterale resolutie gaande van micro- tot nanoschaal. De aangevraagde infrastructuur combinatie is uniek in de Benelux. Het zal de individuele onderzoeksoutput van de verschillende partners in het consortium sterk opschalen, alsook de gemeenschappelijke projecten. Het platform zal de Vrije Universiteit Brussel internationaal weer voorop plaatsen op internationaal niveau.
3. Information on the Flemish universities or university colleges

The number of co-promoters may be adjusted to the situation of the collaboration. Use the available button to add co-promoters to an institution and use the other larger button to add collaborating institutions.

<table>
<thead>
<tr>
<th>Institution</th>
<th>Vrije Universiteit Brussel</th>
</tr>
</thead>
<tbody>
<tr>
<td>Co-promoter</td>
<td></td>
</tr>
<tr>
<td>Full name</td>
<td>Hauffman Tom</td>
</tr>
<tr>
<td>Research Group</td>
<td>Electrochemical &amp; Surface Engineering (SURF)</td>
</tr>
<tr>
<td>Street &amp; Nr.</td>
<td>Pleinlaan 2</td>
</tr>
<tr>
<td>Postal Code</td>
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<tr>
<td>Town</td>
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</tr>
<tr>
<td>Tel.nr.</td>
<td>+32 2 692 35 38</td>
</tr>
<tr>
<td>Email</td>
<td><a href="mailto:tom.hauffman@vub.ac.be">tom.hauffman@vub.ac.be</a></td>
</tr>
<tr>
<td>Status</td>
<td>Post-doc (10% ZAP from January 2016)</td>
</tr>
</tbody>
</table>

| Co-promoter |                           |
| Full name   | Claeys Philippe           |
| Research Group | Analytical, Environmental & Geo-Chemistry (AMGC) |
### Hercules Foundation - Call 2015 -
Medium-Scale Research Infrastructure- with a minimum value of EUR 150,000 and a maximum of EUR 1,000,000 including the non-refundable portion of the VAT

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<td>Email</td>
<td><a href="mailto:phclaeys@vub.ac.be">phclaeys@vub.ac.be</a></td>
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<tr>
<td>Status</td>
<td>Gewoon Hoogleraar</td>
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### Co-promoter

Full name: Snoeck Christophe  
Research Group: Analytical, Environmental & Geo-Chemistry (AMGC)

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<td>+32 2 629 14 80</td>
</tr>
<tr>
<td>Email</td>
<td><a href="mailto:christophe.snoeck@vub.ac.be">christophe.snoeck@vub.ac.be</a></td>
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<tr>
<td>Status</td>
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</tbody>
</table>
### Hercules Foundation - Call 2015 -
Medium-Scale Research Infrastructure- with a minimum value of EUR 150,000 and a maximum of EUR 1,000,000 including the non-refundable portion of the VAT

#### Co-promoter

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<tr>
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<th>Denayer Joeri</th>
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<tr>
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<td>+32 2 629 17 98</td>
</tr>
<tr>
<td>Email</td>
<td><a href="mailto:joeri.denayer@vub.ac.be">joeri.denayer@vub.ac.be</a></td>
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#### Co-promoter

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<td>Tel.nr.</td>
<td>+32 2 629 33 18</td>
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<tr>
<td>Email</td>
<td><a href="mailto:jcousins@vub.ac.be">jcousins@vub.ac.be</a></td>
</tr>
<tr>
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**Co-promoter**

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<th>Van Assche Guy</th>
</tr>
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<td>Physical Chemistry &amp; Polymer Science (FYSC)</td>
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<tr>
<td>Tel.nr.</td>
<td>+32 2 629 39 41</td>
</tr>
<tr>
<td>Email</td>
<td><a href="mailto:gvassche@vub.ac.be">gvassche@vub.ac.be</a></td>
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<td>Hoofddocent</td>
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**Co-promoter**

<table>
<thead>
<tr>
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<th>Nys Karin</th>
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<tr>
<td>Research Group</td>
<td>History of Art &amp; Archaeology (SKAR)</td>
</tr>
<tr>
<td>Street &amp; Nr.</td>
<td>Pleinlaan 2</td>
</tr>
</tbody>
</table>
Postal Code 1050

Town Brussel

Tel.nr. +32 2 629 25 87

Email Karin.Nys@vub.ac.be

Status Hoogleraar

Full name not applicable

Position

Organisation

Research Group/Department

Street & Nr.

Postal Code

Town

Tel.nr.

Email

Main activity of the organisation (public or private research institution, company, etc.)

not applicable
4. Information on the third parties involved (if applicable)
5. Requested financing

5.1. Depreciation period

In principle the depreciation period applicable to the requested infrastructure is 5 years, with the exception of ICT equipment (hardware and software (including databanks), for which the depreciation period is 3 years.

- 5 years
- 3 years

Overview of the consortium

The abbreviations included in the table below will be automatically included in the tables on the next pages. The number of boxes for institutions/third parties provided in the application form is purely indicative.

<table>
<thead>
<tr>
<th>Full name</th>
<th>Abbreviation</th>
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<tbody>
<tr>
<td>Promotor/Institution 1</td>
<td>Vrije Universiteit Brussel</td>
</tr>
<tr>
<td>Institution 2 / Third Party</td>
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<tr>
<td>Institution 3 / Third Party</td>
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<tr>
<td>Institution 4 / Third Party</td>
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<td>Institution 5 / Third Party</td>
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<td>Institution 6 / Third Party</td>
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<tr>
<td>Institution 7 / Third Party</td>
<td></td>
</tr>
<tr>
<td>Institution 8 / Third Party</td>
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</tbody>
</table>

5.2. Requested financing

5.2.1. The eligible costs for funding

The total amount of the eligible costs for the acquisition of the requested equipment/infrastructure (grant exempt from overhead deduction).

*** The 15% rule applies to the costs given under A3., A4. and C3. (see notes).

Each of the specified costs must be justified (obligatory annex in PDF):
- for the investment costs (acquisition, construction, maintenance agreements, upgrades, etc.), add at least one price quotation. Composite amounts must be broken down with a reference to the corresponding amount from the quotation(s);
- for the personnel costs, add an estimate of the personnel costs, if applicable stating the number of man-months expressed in full-time equivalents.
## Eligible costs (in Euro)

<table>
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<tr>
<th>Eligible costs</th>
<th>VUB</th>
<th>Total</th>
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<tbody>
<tr>
<td>A. Costs of scientific investments</td>
<td>929,673,30 €</td>
<td>929,673,30 €</td>
</tr>
<tr>
<td>A1. Costs of the acquisition of infrastructure</td>
<td>929,673,30 €</td>
<td>929,673,30 €</td>
</tr>
<tr>
<td>A2. Costs of components for the construction of the intended research infrastructure</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A3. Repair costs ***</td>
<td></td>
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<tr>
<td>A4. Costs of modifications to buildings and connection costs of research infrastructure ***</td>
<td></td>
<td></td>
</tr>
<tr>
<td>B. Personnel costs for the development and construction of the research infrastructure</td>
<td></td>
<td></td>
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<tr>
<td>C. Maintenance and other costs during the depreciation period</td>
<td>12,342,00 €</td>
<td>12,342,00 €</td>
</tr>
<tr>
<td>C1. Costs arising from maintenance agreements</td>
<td>12,342,00 €</td>
<td>12,342,00 €</td>
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<tr>
<td>C2. Upgrades of research infrastructure</td>
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<tr>
<td>C3. Personnel costs for the permanent maintenance and operation of the research infrastructure ***</td>
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<tr>
<td><strong>TOTAL ELIGIBLE COSTS</strong></td>
<td>942,015,30 €</td>
<td>942,015,30 €</td>
</tr>
</tbody>
</table>
5.2.2. Co-financing by the institutions (Flemish universities, university colleges, strategic research centres and institutions for post-initial education)
Specify the manner in which the percentages of the costs not covered by Hercules will be financed by each partner (= origin of the co-financing provided by the institutions submitting the application (only numbers are allowed in column 2)). Give in column 3 more details about the co-financing by specifying the cost category (see table above A1, A2, A3, A4, B, C1, C2 or C3).

The number of institutions is not limited.

<table>
<thead>
<tr>
<th>Institution (abbrev.)</th>
<th>Contribution</th>
<th>Explanation</th>
</tr>
</thead>
</table>

5.2.3. Contributions by third parties
If third parties are involved in the application, specify here the financial, material and/or personal contribution of each third party. If (a part of) the contribution of one or more third parties is made in kind, in the form of a material or personal contribution, specify how the corresponding equivalent financial value is estimated.

The number of third parties is not limited.

<table>
<thead>
<tr>
<th>Third party</th>
<th>Contribution</th>
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</table>


5.2.4. Summary of the requested financing

In the table below, the names and eligible costs are reproduced from information in the table under 5.2.1. You cannot change this information here. The total subsidisable costs are then calculated when you add the co-financing to the table.

<table>
<thead>
<tr>
<th></th>
<th>VUB</th>
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<td>contribution by third party/ies</td>
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</table>
6. Agreement of the receiving institution

‘The representative of the receiving institution hereby declares his agreement with this project application, in particular with the elements relating to the financing and housing’

Full Name

________________________________________________________________________

Position

________________________________________________________________________

Date

________________________________________________________________________

Signature

________________________________________________________________________
Annexes to be returned with the e-form

- Scientific CV of the promoter-spokesperson and of the co-promoter(s) (PDF file)
- Ethical Advice (if applicable)
- Price quotation(s) for the investment costs (in English)
- Estimate of the personnel cost
- Signature of the promoter-spokesperson
- Agreement of the receiving institution
- Letter(s) of commitment (if applicable)

Save this form and send it with the obligatory annexes by e-mail to RD.secretariaat@vub.ac.be

The final submission date is 14 September 2015 at 12:00 noon