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IUPAC Technical Report

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Abstract: The use of Latin origin terms, relevant for sample characterization modalities, is described with a focus on samples under controlled conditions, samples within devices, and samples during physico-chemical evolution. The terms *in vitro*, *in vivo*, *in situ*, *ab initio*, *in silico*, *post mortem*, *ex situ*, *posthumous*, *in vacuo*, (*in operando*, *post facto*, and *ex post facto*, as used in the scientific literature, are considered. Uses of the Latin origin terms *in situ*, *extra situm*, *in operando*, *in vivo*, *in vacuo*, *in vitro*, *extra vivum*, *post facto* and *ex post facto*, *ab initiis*, *computatro*, and *post mortem* are discussed. It is suggested that these terms are to be used without hyphenation and that all Latin derived terms are set in italic font.

Keywords: *ab initio*; *ex post facto*; *ex situ*; *in silico*; *in situ*; *in vacuo*; *in vitro*; *in vivo*; non-ambient; *operando*; *post facto*; *posthumous*; *post mortem*; sample characterization.

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1 Introduction

There are discrepancies in terms used to describe sample characterization conditions and modalities, even within research communities studying similar systems under similar conditions. This is particularly evident for samples in which the immediate surroundings of the sample are controlled (“non-ambient” conditions), within systems/devices, and undergoing change. The rise of new and conflicting terms occurred in parallel with new sample characterization approaches made available through advances in instrumentation, shifting measurement modalities away from more conventional measurements of samples at equilibrium, toward time-resolved measurements of samples under non-equilibrium conditions, and in more complex surroundings. Commensurate with this shift is the evolution of language and terms used to describe such measurements, which at the broadest level have been referred to generally by communities as “non-ambient”, but really encompass a wider range of sample measurement modalities. This work provides direction for the use of Latin and terms of other origin used to describe the details of the characterization of samples, serving as a basis for consistent language for communities to discuss sample characterization modalities (see Table 1). Section 4 provides a technical commentary on Latin and other origin terms for measurement modalities, which may be of interest as well as help inform decisions about their use and future development. This work is a product of a multidisciplinary collaboration of researchers in chemistry/physics and in Latin language and its historical development. It is recognized that although some terms here may be considered as linguistically incorrect from the historical

Table 1: Sample characterization modalities and typical terms used to describe them.

Characterization modality	Term(s)
Sample at steady state under ambient conditions	No term used
Sample at steady state and held at a particular environmental parameter within a controlled environment such as a sample environment device. Examples: An electrode material within a battery; a sample held at a particular temperature within a cryostat; a sample sealed in a closed vessel, protected from the external environment.	<i>in situ</i>
Sample after modification. Example: An electrode material modified in a battery and then extracted for characterization; a catalyst removed from a catalytic reactor after use and characterized externally.	<i>ex situ</i> <i>post mortem</i> <i>posthumous</i>
Sample not at steady state under non-equilibrium and non-ambient conditions. Example: An electrode material within a battery during cycling of the battery; a working catalyst inside a catalytic reactor under reaction conditions.	<i>in operando</i> <i>operando</i>
Sample under vacuum.	<i>in vacuo</i>
Sample probed by several typically separate characterization tools at the same time. Example: Simultaneous imaging and diffraction characterization of a material.	Multimodal
Sample probed in parts of a larger sample. Example: An electrode material within a series of gauge volumes within a battery.	Mapping Spatially resolved
Sample characterized after modification without being removed from the environment used for modification. Example: An electrode within a battery after cycling.	<i>post facto</i> <i>ex post facto</i>
Sample, usually biological, characterized inside a living system. Example: Cells in a plant.	<i>in vivo</i>
Sample, usually biological, characterized outside a living system. Example: Cells in culture.	<i>in vitro</i>
Quantity or qualitative characteristic that is calculated, sometimes from first principles. Example: Computational calculation of a molecular structure.	<i>ab initio</i>
Quantity or qualitative characteristic that is calculated (by a computer).	<i>in silico</i>

perspective, they have garnered substantial use and meaning within particular communities and their use may not change as a result of the commentary provided.

Experiments are tailored to target specific information within a system, and a number of factors and considerations contribute to achieving desired conditions for characterization of a sample.

- (1) Is the sample being probed as part of a system where the other components are of importance? The matrix may be of the same composition as the sample, such as for spatially resolved characterization.
- (2) Is there an environmental parameter of the sample being controlled such as within a sample environment device?
- (3) Is the sample a closed system or are there input/output components and is the sample changing in response to these?
- (4) Is the sample steady state or changing in response to an environmental parameter and is non-equilibrium?

2 Glossary

2.1 Terms

This section provides definitions for terms used in sample characterization, in the context of this Technical Report. The terms considered include those that have slightly different definitions in the broader chemistry fields as well as those used predominantly within sample characterization specifically.

System. Part or phenomenon of the perceivable or conceivable universe consisting of a demarcated arrangement of a set of entities and a set of relations between these entities, see entry 3.73, [1].

In the present context, the system is the sample, matrix, and any components added or removed during an experiment.

Sample. Material being studied.

Note: Analytical sample is defined as: Sample, taken and, if need be, prepared from a laboratory sample, portions of which are subject to chemical analysis, see entry 3.65, [1].

Matrix. Materials and components within the surroundings of the sample. The matrix may enable the characterization or function of the sample.

Note: In chemical analysis, matrix is defined as: Analytical sample excluding the analyte, with the note: In matrix reference material, the concept “matrix” is used in the sense of a kind of material, see entry 3.44, [1].

Environmental parameter. Condition of the sample such as temperature, pressure, magnetic field, electric field, etc., that is controlled or measured.

Sample environment device. Device that controls an environmental parameter such as a furnace.

Component. Part of a system, see entry 3.24, [1].

Input component. Component that is added to a system including the sample, such as a reactant or carrier gas.

Output component. Component that is removed from a system, including the sample, such as a product of a chemical reaction.

Steady state. State of a system in which one or more characteristics do not change with time, see page 2298, [2]. The use of steady state without qualification of the characteristic implies constant composition and structure. Steady state does not necessarily imply thermodynamic equilibrium.

Non-equilibrium. State of a system that is changing with time, such as undergoing a reaction, see page 175, [3]. Not in a steady state.

Ambient. Uncontrolled immediate surroundings of the system.

While relatively close to the Oxford English dictionary (OED) definition 1.a “That surrounds or encircles; that lies on all sides of something; encompassing” [4], this definition differs slightly from standard definitions found in chemistry fields such as atmospheric chemistry, see page 2173 [5], and also from that defined in the CRC handbook of chemistry and physics [6].

3 Background and history

There has been a growing use of Latin terminology and phrasing over time in the scientific literature. Coupled with this is a lack of consistency in the use of such terms. Over the past few decades, an increasing number of research studies, particularly in materials science, have dealt with new analytical approaches allowing the investigation of a sample under specific conditions.

To describe such sample conditions, Latin origin expressions such as *in situ* and *operando* (also used in the form *in operando*) were introduced. The first of these two expressions was introduced in the beginning of the 20th century, and a consistent growth of use can be dated back to the late 1800s. At that time, it was employed mainly in the fields of engineering related to oil extraction and geological surveys, or in medicine, to designate analyses made, for example, inside an oil well or within a living body. A steady growth of the use of *in situ* is registered around 1985 (Fig. 1), when it first gained use mainly in materials science, specifically in the field of heterogeneous catalysis. Indeed, such catalyst materials are usually treated by heating under a controlled atmosphere, and the sample is compositionally altered by exposure to ambient air which may contain variable amounts of water (moisture). It is therefore necessary to control the environmental conditions of such samples during a characterization study, with such conditions termed *in situ*. From the field of heterogeneous catalysis, this term evolved over time and is now widely applied in most fields of materials science. The development and use of *in situ* evidently triggered the use of the counter expression *ex situ*, to describe the sample condition where the environmental parameters of heat and atmosphere were no longer controlled.

Use of the term *operando* to describe sample characterization originates from the field of heterogeneous catalysis, in response to the need to describe the condition where the sample was under application, in studies aimed at understanding the sample’s working structure. The use of this term was first proposed at the 220th American Chemical Society National Meeting in Washington, DC (August 2000), as testified in “Snapshots of a working catalyst: possibilities and limitations of *in situ* spectroscopy in the field of heterogeneous catalysis” [7], as well as in a review about the importance of such studies in unveiling the structure of active sites in heterogeneous catalysis [8]. The term *operando* was “proposed as an alternative to *in situ* by Miguel Banares (Spanish National Research Council, Institute of Catalysis and Petrochemistry) during a lively discussion with Eric Gaigneaux,

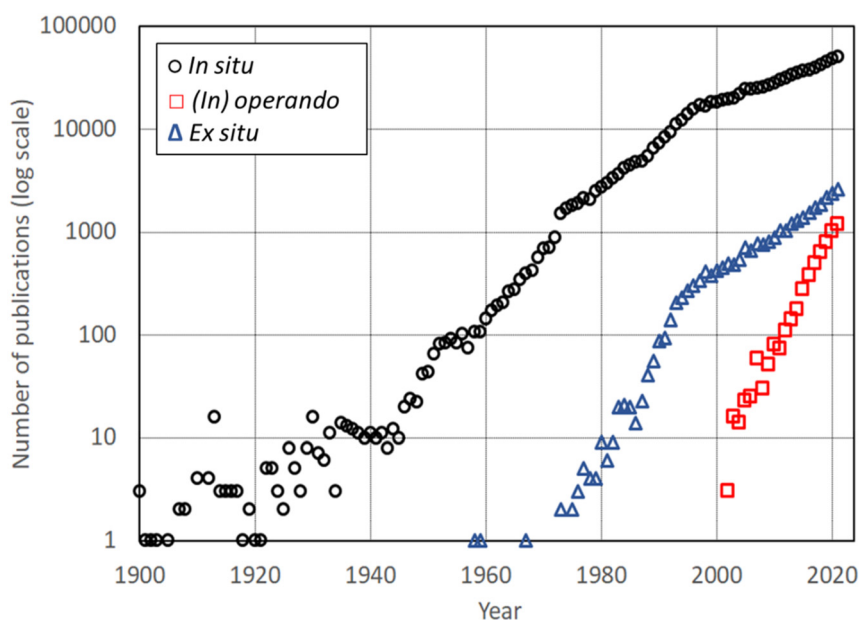


Fig. 1: Use of the expressions *in situ*, *ex situ*, and *(in) operando* in the scientific literature over time until 2021 (Source Scopus).

Table 2: Popularity of terms considered in Section 4 thought to be of Latin origin in research article titles, abstracts, and keywords (Scopus, August 2022).

Expression	Number of publications	First appearance of term in the search as it relates to a sample
<i>in vitro</i>	2 449 841	1903 [10]
<i>in vivo</i>	1 250 838	1896 [11]
<i>in situ</i>	912 343	1874 [12]
<i>ab initio</i>	143 174	1922 [13]
<i>in silico</i>	79 645	1990 [14]
<i>post mortem</i>	41 407	1892 [15]
<i>ex situ</i>	29 930	1958 [16]
<i>posthumous</i>	7024	1945 [17]
<i>in vacuo</i>	6674	1833 [18]
<i>operando</i>	6433	2002 [7]
<i>in operando</i>	1514	2004 [9]
<i>post facto</i>	2413	1970 [19]
<i>ex post facto</i>	1997	1950 [20]

Gerhard Mestl, and Bert Weckhuysen” [7]. *Operando* spectroscopy in its original definition is “the shortened version of spectra of an *operando* or a working catalyst” [7]. The form *in operando* emerged in 2004 [9], with both forms rapidly increasing in use since their introduction and extending to other fields of materials science, with *in operando* rising at a faster rate.

Other terms more commonly used in science now, such as *in vivo*, were only relatively recently introduced to the language of science, despite use by medieval writers and philosophers with other meanings. Further terms, including some derived from Latin, have emerged to describe the conditions of samples under study. A combined search of the Scopus database of both hyphenated and non-hyphenated terms used in research communities, as shown in Table 1, was performed and is shown in Table 2.

4 Latin derivation and usage of terms

See Table 1 for descriptions of characterization modalities of terms in the scientific literature against which a commentary is made below. Where examples are given, they are reproduced exactly as formatted from the publication, including differences in hyphenation, italicization, and use. Terms AD and CE refer to the global standard for the measurement of date *Anno Domini* and Common Era, respectively.

In situ, ex situ

Examples:

- “In most laboratories, *ex situ* techniques are always undertaken to investigate the failure modes of lithium ion batteries” [21].
- “To avoid the possible reactions between sample and air, various *in situ* devices were designed to study the structure changes and interface evolutions during electrochemical cycles” [21].
- “Li foil surface thickness changes were determined by *in-situ* spectroscopic ellipsometry” [22].
- “Recently, *in situ* reaction monitoring using dedicated techniques was shown to be well-suited for the identification of intermediates and to obtain kinetic insights” [23].
- “Passive sampling can be applied in the field (*in situ*) or under controlled laboratory conditions (*ex situ*)” [24].

Comment:

Situs means the “position” of something, or “the particular position occupied by a thing, its site” (OLD “*situs*” 1, [25]). Both *in situ* and *ex situ* are prepositional phrases that combine this word with the prepositions *in* (“in”) and

ex (“out of”) to describe something that is either in or out of a certain specific environment. The phrase *in situ* is not found in Classical Latin (i.e., Latin before approximately 200 AD) but is first found in the 4th century CE from Augustine onward (according to the LLT [26]) and becomes common in Medieval Latin to express the notion of “within something.” There are no examples of the phrase *ex situ* in Classical Latin either, but there are a few occurrences in later times. *In situ* may be used to indicate something which is in its own place or proper position or in a certain place or position. On the other hand, *ex situ* seems not to refer to something departing from its own place or condition (the nuance of “*ex*”), but it is rather used in various expressions conveying the sense “according to (the position of)” or “based upon” etc. Therefore, the proposed definition of *in situ* to describe something within its normal place or condition (e.g., an electrode within a battery) would be correct Latin. As to *ex situ*, there are no surviving examples of this phrase in Latin texts written up to modern times conveying the sense of something being “outside its normal place or condition” (e.g., an electrode extracted from a battery). Theoretically, the phrase may well be used to convey the opposite of *in situ*, but that would depend on the verb used with it, and *extra situm* (attested once in the 1st century CE and twice in the 14–15th centuries CE, according to the LLT [26]) would be a better option, as it is unambiguous.

Operando, in operando

Examples:

- “Neutron powder diffraction (NPD) provides unique and useful information concerning the structure–function relation of battery components and can be used to study the changes to component phase and structure during battery cycling, known as *in operando* measurement studies” [27].
- “While there are many *in situ* and *operando* studies^{10–13} involving spectroscopy, structural, chemical, and surface characterization tools” [28].
- “*Operando* and *in situ* techniques are becoming mandatory to study Li-ion, post Li-ion, and solid-state batteries” [29].
- “*Operando* X-ray absorption and quasi *in situ* X-ray photoelectron spectroscopy revealed that the Cu surface speciation showed a strong dependence on the anolyte concentration” [30].
- “*In-situ/operando* scanning transmission soft X-ray microscopy (STXM), which allows measuring the unoccupied electronic structure with 25 nm spatial resolution in the presence of liquids or reactant gases” [31].
- “This requires *in situ* or *operando* measurements sensitive to the aforementioned sample changes” [32].

Comment:

In operando literally means “in a state of activity” (literally “in [a state of] being busy”); the meaning of the verb *operor* is “to busy oneself, to be at work” (OLD “*operor*” 1, [25]). The grammatical form of both *operando* and *in operando* is the ablative of the gerund (“-ing” verbal noun), without or with the accompanying preposition “*in*”, respectively. The verb *operor* is found in Latin from the archaic period onward and is common. However, *operando* as an ablative gerund without a preposition is not classical usage, albeit rarely found in the Latin of the Roman imperial period. Classical usage would favor the form *in* + gerund, thus *in operando* and not *operando* would be preferred. No specific examples of *in operando* are found in Classical Latin either, but according to the LLT [26], it is used from the 4th century CE onward and becomes common in the Middle Ages. The grammar point at issue is that the ablative case of a gerund (“being busy”) takes a preposition. An ablative gerund can appear without a preposition when it conveys means, cause or manner, but this is not what a phrase is communicating if it describes the sample being measured in a state of activity. There is maybe some small ambiguity in using *operando* without the preposition *in*, as it may suggest “because of being in a state of activity” (cause), or “by being in a state of activity” (means), or describe the adverbial manner or circumstance in which an action took place. It is unambiguous in meaning with the preposition *in*. We therefore suggest using *in operando* rather than *operando*, in spite of the prior introduction of the term *operando* in the scientific literature (*vide supra*).

In vivo

Examples:

- “Since *in vitro* studies cannot entirely predict the influence the drug will have on organs and organ systems, or even the interaction with other drugs, *in vivo* studies are needed to clarify data concerning therapeutic drugs before clinical trials are carried out” [33].
- “*In vivo* calcium imaging from axons provides direct interrogation of afferent neural activity” [34].

Comment:

In vivo is a prepositional phrase combining the preposition *in* (“in, on, among”) and the neuter of the adjective *vivus -a -um* (“living, alive”). It literally means “in a living thing.” As an adjective the term *vivus* generally means “living”; as a noun it can indicate living beings, a living man in the masculine form *vivus, -i*, a living thing in the neuter *vivum, -i* (see L&S “*vivus*”, [35]; OLD “*vivus*”, [25]). From the point of view of Latin usage, the expression is perfectly suited to evoke anything related to living beings such as cellular materials.

In vitro

Examples:

- “*in vitro* studies are critical to the drug development process due to their ability to provide a basis for predicting the clinical results of a drug, including the success or failure of the drug *in vivo*” [33].
- “The two-plasmid approach was used for all *in vitro* characterization, while the bicistronic approach was used for *in vivo* characterization” [34].

Comment:

Vitrum in post-classical and Medieval Latin means both glass and a container made of glass, such as a cup or a glass (OLD “*vitrum*” 1, [25]; L&S “*vitrum*” I, [35]; Du Cange “*vitrum*”, [36]; DMLBS “*vitrum*” 1, [37]). The expression can be used to describe anything that is preserved or grows inside a glass receptacle. With respect to manipulation outside of a living entity, the correct Latin phrase would be *extra vivum*, comprising the preposition *extra* (“beyond the boundaries of”) and the neuter accusative form of the adjective *vivus -a -um* (“living, alive”).

In vacuo

Examples:

- “*In vacuo* X-ray photoelectron spectroscopy (XPS) integrated with the ALD reactor was employed to monitor the chemical changes of the investigated Li surface” [22].
- “The organic layer was dried over Na₂SO₄, filtered and concentrated *in vacuo*” [38].

Comment:

In vacuo is a prepositional phrase combining the preposition *in* (“in, on, among”) and the neuter of the adjective *vacuus* (“empty”). *Vacuus* refers to something (such as places, recipients, etc.) not containing or holding anything, empty (OLD “*vacuus*” 1, [25]). The expression *in vacuo* meaning “in an empty space” and “in the void” is mainly attested from the Middle Ages according to the LLT [26], which contains examples from Thomas Aquinas, William of Ockham, and Roger Bacon, and is frequently used in the language of philosophers, natural scientists and astronomers of the Renaissance, with examples from Galileo Galilei and Christian Wolff. This expression can be used to indicate surroundings devoid of matter or the condition of a sample not surrounded by matter or put into a void space.

Post facto, ex post facto

Examples:

- “In any case, it can be expected that with further application of nanoparticles, both systematic studies and *post facto* analysis of nanoparticles and neurotoxicity will be formulated and become of critical importance to next-generation neuro-nano interfaces” [39].
- “Samples were heated for 40 min with diffraction patterns collected every 20 min and then cooled to room temperature before *ex post facto* diffraction patterns were taken” [40].

Comment:

Post facto is a prepositional phrase, which literally means “after the (or ‘an’) event has taken place” or “after a (or ‘the’) thing has been done.” The nuance of the preposition *post* is “at a time subsequent to, after” (OLD “*post*” 2.2, [25]). The use of *post* with an ablative noun is much less common than with an accusative noun in classical usage. In Classical Latin there are no examples of *post facto*, specifically, but the form is permissible.

Ex post facto is a prepositional phrase which means “in light of subsequent events.” It combines the preposition *ex* (“from,” indicating the source or origin of a phenomenon: OLD “*ex*” 14, [25]) with the ablative of the word *postfactum* “that which is done subsequently.” *Post factum* may appear as one word or as two. *Ex postfacto*

first appears in Late Antiquity in legal texts, from the Digest of Justinian (529 AD) onward, according to the LLT [26].

Both *post facto* and *ex post facto* can be used in the sense of “retroactively” or “because of subsequent occurrence.”

Post mortem

Examples:

- “In order to investigate the distinct degradations of the aged cells, post-mortem analyses were applied to three cells that aged at different voltage values” [41].
- “*Post mortem* or *ex situ* analysis can hardly reveal the stage at which deactivation happens” [32].

Comment:

Post mortem is a prepositional phrase combining the preposition *post* (“after”) and the accusative of the noun *mors* (“death”). The phrase *post mortem* is very common in Latin of all periods. *Mors* is usually used of human or animal death, but it can be used figuratively for the annihilation or extinction of material or immaterial things (OLD “*mors*” 4, [25]). *Post mortem* can be used to describe any action or event taking place “after (the) death (literal or figurative)” of something and its use to describe “spent sample” seems appropriate.

Posthumous

Examples:

- “The *posthumous* analysis was carried out by analysing the electrodes after cycling events such as first charging, first discharging and after 100 cycles” [42].

Comment:

Posthumous is not a Latin term. It derives from *postumus* “last,” “born after the father’s death,” via a folk etymology from *post* (“after”) and *humus* (“ground”). The Latin word *postumus* is the superlative degree of the adjective *posterus* “occurring later”; it is common in Latin of all periods, especially as the name given to a son born after the death of his biological father. *Posthumous* is used in a similar way to *post mortem*, with the latter term being more consistent with its linguistic origins.

Ab initio

Examples:

- “To probe the nature of the possible solid products, *ab initio* random structure searching (AIRSS) is carried out for various $\text{Li}_x\text{S}_{1-x}$ compounds” [43].

Comment:

Ab initio is a prepositional phrase combining the preposition *ab* (“from”) and the ablative of the noun *initium* (“beginning, commencement”). The phrase *ab initio* is very common in Latin of all periods. Cicero uses the word *initium* (in the plural form *initia*) to mean “first principles,” and so the phrase *ab initiis* would be correct Latin expression for “from first principles” using these terms. However, the specific phrase *ab initiis* is not found in this specific sense. *Ab initio* can be used to describe any action or event taking place “from the beginning,” referring to time. If the intention is to mean “first principles,” the phrase *ab initiis* would be the correct form, although no examples of *ab initiis* are found.

In silico

Examples:

- “Such modular approaches offer great promise for automated *in silico* design and, via automated synthesis, also for *in vitro* experiments in catalysis” [44].
- “Through systematic *in silico* transcription factor perturbation in the developing zebrafish, we simulate and experimentally validate a previously unreported phenotype that results from the loss of *noto*, an established notochord regulator” [45].

Comment:

This phrase does not appear in Classical Latin. There is no Classical Latin word *silicum*. In 19th century scientific Latin, the term *silicium* was coined to describe the newly-discovered element “silicon” (Si); it derives from Classical Latin *silix* meaning “stone” or “flint.” The Latin etymology of the English word “computer” is *computare* “to calculate, count up, reckon” (OLD “*computo*” 1, [25]); perhaps a neologism such as *computatrum* or *instrumentum computatorium* may be closer. The form *in silico* is not attested in Latin; *in silicio* would be comprehensible to describe something made or designed on a computer, but the more expected phrase would be *in computatro* or *e computatro*, or simply *computatro*. No examples of *computatro* are found in the literature.

5 Style conventions

Both hyphenated and non-hyphenated terms appear in the literature, as well as a mixture of italicization for Latin and other derived terms. Specific journals may have particular style conventions, such as outlined in the American Chemical Society style guide for publications [46], which suggests that Latin terms such as *in situ* and *in vitro* should not be italicized.

It is suggested in this Technical Report that these terms be used without hyphenation and that all Latin derived terms are italicized.

6 Membership of Analytical Chemistry Division 2021–2023

President: David Shaw; Vice President: Derek Craston; Past President: Zoltán Mester; Secretary: Luisa Torsi; Titular Members: Resat Apak, Vasilisa B. Baranovskaia, Jiří Barek, Ilya Kuselman, Takae Takeuchi, Susanne Kristina Wiedmer; Associate Members: Franziska Emmerling, Erico Marlon de Moraes Flores, Ivo Leito, Hongmei Li, Aura Tintaru, Winfield Earle Waghorne; National Representatives: Raychelle Burks, Hye Ryung Byon, Orawon Chailapakul, Jan Labuda, Charles Lucy, M. Clara F. Magalhães, Thalappil Pradeep, Malarvili Ramalingam, Rufus H. Sha’Ato, Danny van Oevelen; Emeritus Fellow: D. Brynn Hibbert.

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