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TECHNICAL REPORT

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Nanotechnologies — Considerations for the development of chemical nomenclature for selected nano-objects

Nanotechnologies — Considérations concernant le développement de la nomenclature chimique de nano-objets choisis

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Foreword

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The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

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For an explanation on the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the WTO principles in the Technical Barriers to Trade (TBT), see the following URL: Foreword - Supplementary information

The committee responsible for this document is ISO/TC 229, *Nanotechnologies*.

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Introduction

For the purposes of this Technical Report, the term *nomenclature* refers to the name and a minimum set of descriptors which are uniquely assigned to a particular nano-object entity or complex. Advanced measurement and instrumentation allows us to "see" at the nanoscale. Measurement tools and techniques are improving our ability to distinguish among nano-objects with the same chemical composition, but which behave differently, based on differences in size, shape or surface functionalization. Yet, the application of established chemical nomenclature systems to describe differences among nano-objects with the same chemical composition has limitations.

For the research and development community, including academia, nomenclature assists in the communication of properties, effects and other relationships or interactions between nano-objects. It also enables effective communication regarding the specific nano-object, which facilitates repeatability of experimental data by other scientists, replication by manufacturers, and application for and protection of patents. For industry and consumer groups, specific names to distinguish nano-objects allow differentiation between products, facilitate patent applications and protect intellectual property rights. Regulators rely on chemical nomenclature to characterize chemical substance and manage the associated environmental and health risks, if and where applicable.

This Technical Report presents an initial effort to support new work Item proposals to pursue chemical nomenclature that is specifically tailored to nano-objects. It identifies categories of nano-objects which could require distinct nomenclature models and discusses essential descriptors to support nano-object nomenclature conventions. A future consideration will be to decide whether to undertake the development of a searchable information system capable of cataloguing a sizable library of names and structural features. This Report also makes recommendations concerning collaboration with existing chemical nomenclature organisations. Finally, this Technical Report considers how the development of nomenclature models for nano-objects will keep pace with and incorporate new science and terminology.

It should be understood that the term "nanomaterials" is broadly defined by ISO to encompass "nano-objects" and "nanostructured materials". In the future, consideration will be given to chemical and nonchemical nomenclature for classes of nanostructured materials, devices and systems at the nanoscale, and strategic application areas.

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Nanotechnologies — Considerations for the development of chemical nomenclature for selected nano-objects

1 Scope

This Technical Report is intended to provide information and analyses in support of the development of chemical nomenclature for the naming of "nano-objects". "Nano-objects" have been defined in ISO/TS 80004-1:2010 to mean "materials with one, two, or three external dimensions in the nanoscale", with the nanoscale defined as the "size range from approximately 1 nm to 100 nm". Nano-objects are further defined as nanoplates, nanofibres, and nanoparticles.

More specifically, the nano-objects that are the subject of this Technical Report are discrete chemical entities rather than devices or mixtures (preparations). The nano-objects discussed in this Technical Report are not intended to constitute an exhaustive list.

This Technical Report is intended to facilitate communications between developers and potential users of nomenclature including academia, industry, government and non-governmental organizations.

2 Normative references

The following referenced documents are indispensable for the application of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO/TS 27687:2008, *Nanotechnologies — Terminology and definitions for nano-objects — Nanoparticle, nanofibre and nanoplate*

ISO/TS 80004-1:2010, *Nanotechnologies — Vocabulary — Part 1: Core terms*

ISO/TS 80004-3:2010, *Nanotechnologies — Vocabulary — Part 3: Carbon nano-objects*

ISO/TS 80004-4:2011, *Nanotechnologies — Vocabulary — Part 4: Nanostructured materials*

3 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO/TS 27687, ISO/TS 80004-1, ISO/TS 80004-3, ISO/TS 80004-4 and the following apply.

3.1
carbon nanotube
CNT
nanotube composed of carbon

Note 1 to entry: Carbon nanotubes usually consist of curved graphene layers, including single-wall carbon nanotubes and multiwall carbon nanotubes.

[SOURCE: ISO/TS 80004-3:2010, definition 4.3]

3.2
fullerene
molecule composed solely of an even number of carbon atoms, which form a closed cage-like fused-ring polycyclic system with 12 five-membered rings and the rest six-membered rings

Note 1 to entry: Adapted from the definition in the IUPAC Compendium of Chemical Terminology.

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Note 2 to entry: A well-known example is C_{60}, which has a spherical shape with an external dimension of about 1 nm.

[SOURCE: ISO/TS 80004-3:2010, definition 3.1]

3.3
nano-object
material with one, two or three external dimensions in the nanoscale

Note 1 to entry: Generic term for all discrete nanoscale objects.

[SOURCE: ISO/TS 80004-1:2010, definition 2.5]

3.4
nanoscale
size range from approximately 1 nm to 100 nm

Note 1 to entry: Properties that are not extrapolations from a larger size will typically, but not exclusively, be exhibited in this size range. For such properties the size limits are considered appropriate.

Note 2 to entry: The lower limit in this definition (approximately 1 nm) is introduced to avoid single and small groups of atoms from being designated as nano-objects or elements of nanostructures, which might be implied by the absence of a lower limit.

[SOURCE: ISO/TS 80004-1:2010, definition 2.1]

3.5
quantum dot
crystalline nanoparticle that exhibits size-dependent properties due to quantum confinement effects on the electronic states

[SOURCE: ISO/TS 27687:2008, definition 4.7]

4 Abbreviated terms

CAS	Chemical Abstracts Service
CAS RN	Chemicals Abstracts Service Registry Number
CNT	carbon nanotube
DEFRA	Department for Environment, Food and Rural Affairs (United Kingdom)
DTSC	California Department of Toxic Substances Control (United States)
DWCNT	double-wall carbon nanotube
EPA	United States Environmental Protection Agency
InChI	International Chemical Identifier
IUBMB	International Union of Biochemistry and Molecular Biology
IUPAC	International Union of Pure and Applied Chemistry
MWCNT	multiwall carbon nanotube
NICNAS	National Industrial Chemicals Notification and Assessment Scheme (Australia)
NIST	United States National Institute of Standards and Technology
NMSP	Nanoscale Materials Stewardship Program, US EPA (United States)

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OECD	Organization for Economic Co-operation and Development
OECD WPMN	Working Party on Manufactured Nanomaterials (OECD)
SMILES	Simplified Molecular Input Line Entry Specification
SWCNT	single-wall carbon nanotube
TSCA	Toxic Substances Control Act, US EPA (United States)
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials

5 Nomenclature

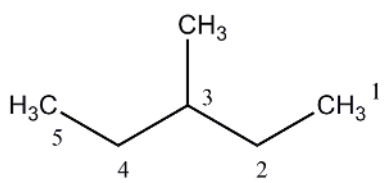
5.1 Nomenclature defined

The term nomenclature is derived from the Latin root "*nomen*" which means "name", while "*clatura*" stems from "Calare", which means to "call" or "summon". Princeton University defines nomenclature as *"a system of words used to name things in a particular discipline"*[6]. For the purposes of this report, *nomenclature* is a system of naming that provides a minimum set of descriptors relevant for the purpose of deriving the name. The name assigned enables its identity to be readily understood.

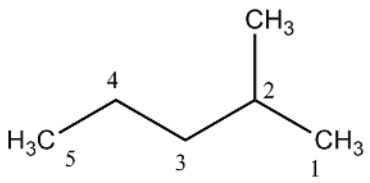
In contrast to nomenclature, *terminology* (or vocabulary) is a body of terms used in a subject of study or profession, etc. Often loosely referred to as "nomenclature", terminology is in fact a list of terms and definitions that ensures a common understanding of the language used in a particular field. An example of terminology would be the definition of the term *nanoparticle* which has been formally adopted by ISO to mean *"a nano-object with all three external dimensions in the nanoscale."*

5.2 Chemical nomenclature

When naming organic chemical compounds, for example, rules are based on naming the chemical's parent structure, as well as the chemical groups attached to the parent structure and their relative positioning. For Compound A (below), the structure is named by first identifying the parent structure (i.e. pentane) and then identifying the substituent group (i.e. -methyl), and its relative position (i.e. attached to the 3rd of 5 carbons in the parent chain). The resulting name for this compound is 3-methyl pentane. A shift of the methyl group to a neighbouring carbon on the parent chain results in a different chemical structure and the name, 2-methyl pentane (Compound B).



Compound A



Compound B

5.3 International Union of Pure and Applied Chemistry (IUPAC) chemical nomenclature

IUPAC has developed and still is expanding a system of rules for chemical nomenclature. In the highly specialized field of chemical nomenclature, IUPAC serves to advance worldwide aspects of the chemical sciences. It develops and provides nomenclature systems which allow chemical compounds to be named uniquely and thereby distinguished from each other. These names represent the composition and structure of the compound. The structure must be known for a unique name to be produced, and that name can then be deciphered to produce a structure. Other than in ways implied by structure or composition, IUPAC nomenclature does not distinguish between molecules based on size, volume, or chemical properties.

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5.4 Chemical Abstracts Service (CAS) chemical nomenclature

CAS is a not-for-profit division of the American Chemical Society which maintains a nomenclature system, closely related to the IUPAC system, for the purpose of database building and information retrieval. The CAS system has nomenclature rules for discrete chemicals, polymers and chemicals of Unknown or Variable Composition, Complex Reaction Products and Biological Materials (UVCB's).

CAS's naming conventions depend on whether the chemical substance has a fixed chemical structure (such as discrete chemicals), a number of repeating units (such as polymers), or is characterized as a UVCB. An example of a UVCB name would be "Chemical A, reaction products with Particle X". This system does not distinguish based on size or volume. However, this system lacks specificity and allows particles of any size, morphology, structure to be encompassed by "Particle X", as well as any degree of reaction of Chemical A on the surface of Particle X.

Both IUPAC and CAS approaches have some useful elements to consider as part of chemical nomenclature for nano-objects, and are further described in Annex A.

6 Chemical nomenclature systems for nano-objects and other relevant approaches

Apart from traditional IUPAC and CAS chemical nomenclature systems, chemical nomenclature proposals that address nano-objects are sparse and most of these proposals address forms of carbon, coinciding with the emergence of new forms of carbon such as fullerenes.

Dresselhaus et al. (1992),[7] introduced vector notation for classifying the atomic structures of single-wall carbon nanotubes (SWCNTs). By using the chiral vector C = (n, m), a SWCNT is called *armchair* type in the case of C = (n, n), *zigzag* type in the case of C = (n, 0), and *helical* type for the other cases. Depending on whether (n-m) is a multiple of 3 or not, the electronic structure of the SWCNT is metallic or semi-conducting. This system, however, does not consider the length of the nanotube or the structure of the nanotube ends. This notation system could be extended for double wall carbon nanotubes (DWCNTs), but would not be realistic for multiwall carbon nanotubes (MWCNTs) with many layers.

IUPAC (1997)[8] has published a preliminary survey of methods for naming fullerenes designed to differentiate between fullerenes based on atom connectivity. However, it does not easily extend (nor was it intended) to apply to non-fullerene nano-objects and complex physical geometries.

Inagaki and Radovic (2002)[9] have proposed a system of nomenclature for nanoscale forms of carbon based on factors controlling the preparation and production process. Factors are classified on the basis of (i) dominant aggregation state during carbonization (i.e. gas, liquid, solid phase); (ii) conditions of processing; and (iii) key structural or textural features of the resulting products. Resulting forms of nanoscale carbon are described as either nanostructured or nano-size. The authors view "nanocarbons" as "carbon materials produced at the nanometer scale" when *either* their size or their structure is controlled. This definition would be therefore applicable to an enormous variety of carbon nano-objects, in addition to fullerenes and nanotubes.

In 2006, ASTM International developed a naming system for carbon black which was intended for the rubber industry.[10] This naming convention differentiates between carbon black species based on curing rate, surface area (rating 0-9), and two arbitrary parameters. This system however, might not encompass the full range of parameters necessary for naming applications of carbon black, nor other forms of nanoscale carbon.

Glotzer and Solomon **(**2007) [11] have proposed a generalized set of anisotropy dimensions to describe key attributes of particles and their interactions. The dimensions are surface coverage (patchiness), aspect ratio, faceting, pattern quantization, branching, chemical ordering, shape gradient, and roughness. The dimensions are intended to be used to describe homogeneous and heterogeneous interactions, especially those involved with aggregation, agglomeration and self-assembly. As emphasis is placed on particle interactions rather than particle composition, some adjustments would be necessary for a nomenclature system for nano-objects.

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Gentleman and Chan (2009)[12] offer an indexing system for use by other academic scientists and recommend using physical parameters coupled with a chemical name to distinguish nano-objects and their larger scale counterparts. Numerical identifiers point to a specific parameter (such as size, shape, core chemistry, ligand, and solubility). The proposed codes include chemical classes (organic/fullerene or inorganic/organometallic), outermost chemistry (dendrimer, fullerene, liposome or polymer), size and shape (ball, polyhedron/faceted, rod/wire, plate/disc/well), core chemistry, ligand chemistry (functional groups attached to inside or outside of nanostructured chemical substances) and solubility (in water or in organic solvents). This coding system is quite unique, but some modifications would be necessary to codify different carbon nanotubes more precisely. For example, it does not discuss the category of "tube" or "hollow fibre". For ligand chemistry, it does not call for the locations of functional groups and it does not specify the numbers, kinds and locations of encapsulated objects.

In 2012, Suarez-Martinez, Grobert and Ewels[13] proposed a system for naming nanoscale forms of carbon that focuses on morphological differences (e.g. single or multiwall, hollow, bundled) and geometrical transformation (e.g. stacked, cut, scrolled, coned) rather than synthesis conditions, physical properties, or texture. They propose to arrange families of forms of graphene in a standardized format expressing their periodic dimension, e.g. molecular form (zero dimensional), cylindrical nanoforms (one dimensional) and layered nanoforms (two dimensional). Their system would propose the name "multi-walled fullerenes" for "multiple-encapsulated closed carbon layer structures" currently referenced as "carbon onions" or "nested fullerenes". In addition, the authors propose nomenclature to identify materials consisting of two or more forms of nanoscale carbon which can be extended to describe the chemical composition of heterogeneous, carbon-based nano-objects.

Thomas et al. (2012)[14] developed a nomenclature system to create computable string expressions that identify and enumerate the different high-level types of material parts of a nanoparticle formulation and represent the spatial order of their connectivity to each other. The goal of this system is to provide descriptions of nanoparticle formulations that not only describe the spatial connectivity of nanoparticle components, but also provides information about the other substances present in the medium in which the nanoparticle is present. These string representations are intended to be both human- and computer-readable, and to be annotated with ontology terms, allowing the structure of the nanoparticles and the composition of the formulation to be reconstructed and interpreted from the identifying string.

These approaches have elements useful to consider as part of chemical nomenclature for nano-objects, and certain of them are further described in Annex B.

7 Survey of nano-objects

7.1 General

As goods move in trade, they are subject to an array of requirements that often include reliance on quality, safety, and other regulations and standards. Streamlining the hurdles for commercial acceptance through harmonized international standards helps to promote an integrated global economy. In recognition of the role of standards in international commerce, a systematic effort was undertaken to establish a "snap shot" of the chemical substances and families of chemical substances that have or are expected to have commercial utility in nanotechnology applications.

For this purpose, surveys of the ISO/TC 229 and IEC/TC 113 membership were undertaken. All member bodies of ISO/TC 229 and IEC/TC 113 were requested to identify and compile chemical information on nano-objects (e.g. nanoparticles, nanofibres, nanoplates, nanotubes, etc), or families of nano-objects (e.g. carbon nanotubes, quantum dots) for consideration in the Nomenclature Framework project (ISO/TC229/JWG1/PG11).

The survey form was designed to capture chemical information on discrete organic and inorganic nano-objects and families of nano-objects. It was not intended for use with pure or compounded biological materials, nanostructured materials larger than the nanoscale (e.g. polymer matrix composite, ceramic matrix composite, nanotextured surfaces) or devices. Member bodies were invited to describe how existing IUPAC or CAS nomenclature applied to the nano-objects nominated in the survey, identify

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drivers for developing nomenclature system, as well as whether existing nomenclature approaches were adequate.

It is acknowledged and understood that the responses to the membership survey might reflect the particular preference by the responding country in a given application area. Moreover, the results of the survey and subsequent analyses are not intended to provide a complete list of all of the chemical substances that are being researched or used in all nanotechnology applications. Some nano-objects including cadmium sulfide and graphene nominated by TC 229/TC 113 members did not qualify for final ranking in Table 1. These are nonetheless important chemistries in certain applications of nanotechnologies.

A total of 28 surveys were received, from 10 countries, describing 16 materials in commerce from ISO/TC229 and IEC/TC 113. A representative summary of the survey responses is included as Annex C.

7.2 Selection of public listings of nano-objects

7.2.1 Introduction

To gain additional chemical information with which to objectively evaluate the potential commercial relevance of nano-objects, a review was undertaken of public lists of chemical substances identified as having commercial relevance in nanotechnology. These lists have been developed by a number of international organizations and jurisdictions in order to facilitate research or assessment prioritization. The identified resources are further addressed in Annex C.

These listings represent classes of nano-objects currently in commerce, as well as materials of interest to regulatory programs. Materials on these lists are considered primarily in the range of 1 nm to 100 nm. These chemical substances can be considered first generation nano-objects but might not be completely reflective of all classes currently in research and development. Furthermore, there was no attempt to canvas the research community beyond the memberships of ISO/TC 229 and IEC/TC 113.

7.2.2 ISO/TC 229 programme of work

ISO/TC 229[15] is pursuing standardization in the field of nanotechnologies. Working Groups have been established in the following areas: terminology and nomenclature, measurement and characterization, health, safety and environmental aspects, and material specifications. To promote coordination among Working Groups within TC 229, the work programme of TC 229 was examined for projects which demonstrate a specific focus on specific nano-objects or classes/subclasses of nano-objects. In addition, the so-called "nano-tree" categorization project provides an interesting perspective on how nano-objects can be organized.

7.2.3 OECD "Guidance Manual for the Testing of Manufactured Nanomaterials"

The OECD-issued list of representative manufactured nanomaterials[16] identifies nano-objects which are in commerce to direct the development of test data particularly in the areas of measurement, toxicology and risk assessment of nanomaterials. Certain nano-objects not included in the list could become important in the future and those currently on the list might have (over time) reduced production and/ or use.

7.2.4 Australian National Industrial Chemicals Notification and Assessment Scheme (NICNAS)

As a result of data from voluntary industry surveys in 2006 and 2008, and in consideration of Australia's involvement in the OECD testing program, NICNAS identified an indicative but not exhaustive list of substances that may be produced as nano-objects in a public discussion paper in November 2009 entitled "Proposal for Regulatory Reform of Industrial Nanomaterials"[17].

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7.2.5 UK Department for Environment, Food and Rural Affairs (DEFRA)

DEFRA commissioned the Institute of Occupational Medicine to undertake a prioritization exercise to identify materials for the development of reference materials for use in research.[18] The resulting REFNANO project is based on an informed discussion and opinion-gathering activity with representatives from toxicology, metrology and the producer/user communities. Based on discussions and recommendations from two workshops, a list of eight high priority nano-objects was established.

7.2.6 US EPA's "Nanoscale Materials Stewardship Program"

In October 2006, EPA launched a collaborative process and invited stakeholders to participate in the design, development and implementation of a Nanoscale Materials Stewardship Program (NMSP).[19] The release of the July 2007 NMSP concept paper, TSCA Inventory paper, and Information Collection Request for the NMSP for public review and comment were part of the collaborative development process. The NMSP had two parts:

— Basic Program for reporting available information on engineered nanoscale materials that were manufactured, imported, processed or used; and

— In-depth Program to voluntarily develop data, including testing, for certain of these nano-objects over a longer time frame.

The voluntary NMSP ended in December 2009. Thirty one organizations covering more than 132 nanoscale materials submitted information under the Basic program.

7.2.7 California Department of Toxic Substances Control Information Call-In

The State of California in the United States has the eighth largest economy in the world. In 2009, the Department of Toxic Substances Control (DTSC) initiated a chemical information call-in for carbon nanotubes and issued a list of additional nano-objects that could be subject to data call-ins in the future.[20] DTSC wants to understand the use of nanotechnology for approaches to green chemistry, pollution prevention, and sustainable manufacturing strategies.

7.2.8 Commercially available data in the Nanowerk Database

Nanowerk is a nanotechnology and nanosciences portal developed and maintained by Nanowerk LLC which, as of 2011, listed over 2,200 nanomaterials commercially available from more than 145 international suppliers of nanomaterials.[21]

7.3 Ranking of surveyed nano-objects

7.3.1 General

Before directing limited resources to initialize the further development of chemical nomenclature systems for nano-objects, it was agreed to develop a critical understanding of what materials are available commercially and which materials are viewed as having the greatest priority for nomenclature development. As a result, a system for ranking the nano-objects and classes of nano-objects that were identified through the ISO/TC 229 and IEC/TC 113 survey and international databases was undertaken. Information gained from this exercise is designed to inform the need for and development of nomenclature for classes of nano-objects generally. The results of this exercise are contained in this Technical Report and are offered to help establish an objective basis for recommendations on chemical nomenclature needs in nanotechnologies.

As previously noted, in 1997 IUPAC published an approach for naming fullerene materials. However, this subclass was made part of the prioritization exercise with a view toward understanding its current level of usage and acceptance within the international community. Moreover, information received in the ISO/TC 229 nomination process represents self-directed responses and as such does not represent a comprehensive assessment of nomenclature needs. Nevertheless, these responses provide highly valuable insight from experts in the field whose experiences and pursuits are challenged by nomenclature

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