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

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National foreword

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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

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

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).

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights. Details of any patent rights identified during the development of the document will be in the Introduction and/or on the ISO list of patent declarations received (see www.iso.org/patents).

Any trade name used in this document is information given for the convenience of users and does not constitute an endorsement.

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*.

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.

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.

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)

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

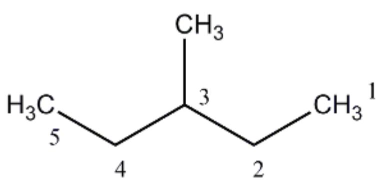
5.1 Nomenclature defined

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.

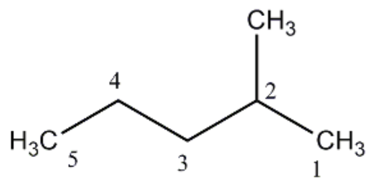
In contrast to nomenclature, *terminology* (or vocabulary) is a body of terms used in a subject of study or profession, etc. Often loosely referred to as "nomenclature", terminology is in fact a list of terms and definitions that ensures a common understanding of the language used in a particular field. 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.

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.

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 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].

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 available chemical nomenclature. With these qualifications in mind, the priorities for chemical nomenclature development identified through this exercise are candidates for proof of concept with respect to nano-object chemical nomenclature system development.

7.3.2 Inclusion in ISO/TC 229 survey

The TC 229 survey captured chemical information on 16 discrete inorganic and organic nano-objects and families of nano-objects. There were 28 responses received from the 10 member bodies that contributed responses. For purposes of understanding the relative degree of interest among member bodies in applications involving the nano-objects identified through this survey, a value of 5 was assigned where at least two member bodies expressed interest in a sub-class of nano-objects[1]. A value of 3 was assigned where a single member body expressed an interest in a sub-class of nano-objects. An additional value of 1 was assigned to a sub-class where at least one member expressed interest in a nano-object belonging to that sub-class.

7.3.3 Consistency with ISO/TC 229 work and level of interest expressed in international information sources

Values also were assigned as a means to gauge the level of coordination of the work of TC 229 with the surveyed interests of member bodies and with the listings of nano-objects among various international public databases with a regulatory focus. A value of 5 was assigned based on the existence of at least 4 work items relating a sub-class of nano-objects in TC-229. A value of 3 was assigned based on the existence of 2-3 work items in TC 229 relating to a sub-class of nano-objects. An additional value of 1 was assigned if there were 0-1 work items in TC 229 relating to a sub-class of nano-objects.

In addition, a value of 1 (i.e. maximum score of 5) was assigned based on the existence of a sub-class of nano-objects in each of the following sources:

— Guidance Manual for the Testing of Manufactured Nanomaterials (OECD);

— “Nanoscale Materials Stewardship Program” (US EPA);

— Australian National Industrial Chemicals Notification and Assessment Scheme (Australia NICNAS);

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

— California Department of Toxic Substances Control (DTSC).

7.3.4 Commercially available as listed in Nanowerk database

Priority rankings were established with and without the commercially-oriented Nanowerk database. A value of 5 was assigned if the material was available from greater than 25 suppliers in the Nanowerk database. A value of 4 was assigned based on a material being available from 11 to 25 suppliers. A value of 3 was assigned based on a material being available from 6 to 10 suppliers. A value of 2 was assigned based on a material being available from 3 to 5 suppliers. Finally, a value of 1 was assigned based on a material being available from less than 3 suppliers.

7.4 Ranking results

7.4.1 Approach taken

The ranking approach undertaken by ISO/TC 229 was designed to cover a wide range of stakeholder interests. First, consideration was given to the specific interests in nomenclature development as expressed by ISO/IEC member bodies and as identified by the ISO/TC 299 work program. Second, external stakeholder interests were identified in international database listings, which tended to be of

1) An expression of “interest in a sub-class of nano-objects” was considered either a direct reference to a broad sub-class by a member organization, or multiple references to nano-objects within a sub-class by a single member organization.

a regulatory interest in nature, and as indicated by their commercial availability for sale in the global marketplace. The needs and interests of the research community in chemical nomenclature for nano-objects were ascertained by identifying scientific publications describing representative nomenclature, indexing, or characterization approaches. Scoring results are presented in Table 1 with and without the Nanowerk data. Results from both approaches share the same top 12 priorities, in the same order. There are 4 subclasses that are unique results to each approach. Overall, these results provide a representative spectrum of the chemical substances of current commercial, regulatory, and scientific interest in nanotechnologies. Nano-object groupings generated by these results have also been suggested with a view toward developing category specific nomenclature systems.

Table 1 — Summary of ranking results

	Without Nanowerk Data		With Nanowerk Data	
Ranking	**Nano-object**	**Score**	**Nano-object**	**Score**
1	SWCNT***	16	SWCNT***	21
2	MWCNT***	15	MWCNT***	20
3	Titanium Dioxide**	13	Titanium Dioxide**	18
4	Silver Nanoparticles*	11	Silver Nanoparticles*	16
5	Fullerenes***	10	Fullerenes***	15
6	Silicon Dioxide/Silica**	9	Silicon Dioxide/Silica**	14
7	Gold Nanoparticles*	8	Gold Nanoparticles*	14
8	Iron Oxide**	8	Iron Oxide**	13
9	Cerium Oxide**	7	Cerium Oxide**	12
10	Copper Nanoparticles*	7	Copper Nanoparticles*	12
11	Zinc Oxide**	6	Zinc Oxide**	11
12	Nano Diamond***	5	Nano Diamond***	9
13	Nanocellulose****	4	Calcium Carbonate****	9
14	Aluminium Oxide**	3	Aluminium Oxide**	8
15	Quantum Dots*****	3	Nickel Nanoparticles*	8
16	Carbon Black***	3	Quantum Dots*****	8
17	Nanoclays*****	3	Copper Oxide**	7
18	Zero Valent Iron*	3	Magnesium Oxide**	6
19	Nickel Nanoparticles*	3	Aluminium Nanoparticles*	6
20	Magnesium Oxide**	3	Zirconium Oxide**	6

* noble metals; ** metal oxides; *** elemental carbon; **** organics; ***** others: quantum dots, nanoclays

7.4.2 Description of metals (elemental) grouping

Metal nanoparticles ranked to be of current high interest in nanotechnology applications include gold (Au), silver (Ag), copper (Cu), nickel (Ni), and zero valent iron (Fe). These are available in a wide variety of shapes (e.g. spheres, rods, wires, cubes, prisms) and can be part of a core-shell structure or composite material. It is recognized that size, size distribution, surface chemistry, and surface charge can contribute to changes in the performance properties of these nano-objects. This grouping also can be referred to as plasmonic nanoparticles or nanostructures due to their ability to sustain surface plasmon resonance. Current chemical nomenclature systems describe their molecular connectivity and are not intended to describe these nano-objects in the context of their size, shape or properties.

7.4.3 Description of metal oxides grouping

Metal oxides that were identified as high ranking in terms of applications in nanotechnology include titanium dioxide, silicon dioxide, iron oxide, cerium oxide, zinc oxide, copper oxide, aluminium oxide, magnesium oxide, and zirconium oxide. These nano-objects have varying properties based on size, surface chemistry and functionalization, core-shell interactions, crystalline state, surface area and polymorphism. In the case of iron oxide, different species (Fe_2O_3 and Fe_3O_4) have different properties and in the 2 nm to 20 nm range these materials can also be superparamagnetic. These nano-objects are finding utility in magnetic confinement assays, biological imaging (magnetic resonance) and sequestration applications. CeO_2 nanoparticles are involved in, for example, catalysis applications (diesel motor), fuel cell technologies, and coating applications (for mechanical stability and hardness).

The current chemical nomenclature systems predominantly describe molecular connectivity. For titanium dioxide generally, chemical nomenclature systems recognize the anatase, rutile and brookite forms. However, the systems are not intended to describe these nano-objects in the context of size or other parameters which may lead to changes in expressed properties.

7.4.4 Description of carbon grouping

Nano-objects of carbon identified through this ranking approach include fullerenes, SWCNTs, MWCNTs, carbon black, and nanodiamond. Carbon-based fullerenes comprise various cage-like, hollow molecules composed of hexagonal and pentagonal groups of carbon atoms. Carbon nanotubes vary in properties according to number of walls (single, double, multi, etc), chirality, manufacturing processes, and impurities. Carbon black is virtually pure carbon in the form of aggregated particles that are produced by incomplete combustion or thermal decomposition of gaseous or liquid hydrocarbons under controlled conditions. Its physical appearance is that of a black, finely divided pellet or powder. Its use in tires, rubber and plastic products, printing inks and coatings is related to properties of specific surface area, particle size and structure, conductivity and colour. Carbon black is among the top 50 industrial chemicals manufactured worldwide, based on annual tonnage. The nanodiamond subclass can be typically described as polycrystalline diamond films that can vary in properties depending on thickness of carbon shell, graphitization level, particle agglomeration, etc. Applications for nanodiamonds open a way to substantial improvement of the characteristics of abrasive and polishing compositions, lubricants, abrasive tools, polymer compositions, resins and rubbers, magnetic recording systems, and provide a possibility of growing diamond films on a variety of substrates.[2)]

CAS and IUPAC nomenclature systems for carbon nano-objects predominantly describe molecular connectivity, similar to other classes. No new considerations for nomenclature for carbon black have been identified. Chemical nomenclature for fullerenes permits these nano-objects to be differentiated. As noted elsewhere, proposals have been put forward to describe carbon nano-objects based on manufacturing process, structure, and morphology. However, a harmonized and comprehensive system for naming and distinguishing among CNTs, in particular, is lacking at this time. Nanodiamond also lacks a dedicated system of nomenclature.

7.4.5 Description of core-shell structures

The survey exercise identified a number of core-shell nanoparticles which would benefit from a nomenclature system. Quantum dots, which are semiconductors and display size-dependent properties on the nanoscale, are typically core-shell structures and currently cannot be adequately distinguished using conventional, chemical-based nomenclature. Similarly, cadmium sulfate is a core-shell structure which consists of a quasi-spherical core, such as cadmium (Cd) chalcogenide, 2 nm to 20 nm in diameter, surface functionalized with a phosphorus (P) or sulfur (S) poly-oxo-anion, such as hexametaphosphate,

2) The predominant subclasses of elemental carbon are recognized to include graphene, formed from individual layers of sp^2 carbon that can vary in properties based on molecular order and porosity. Agglomerates formed from highly ordered 3-D forms of graphene can differ significantly from intercalates of graphite in terms of the porosity and order that can be achieved. The combined effect of order and porosity on a molecular scale has been shown to significantly affect properties such as tensile strength, conductivity, surface area and electro-magnetic properties in certain instances. Since the original survey and ranking exercise was performed, molecular graphene has come to be referenced as a nano-object much in the way of fullerenes.

tripolyphosphate, or thiosulfate. The ionized oxygen (O) provides a stabilizing negative charge (in an aqueous medium) for the nanoparticle and the P or S binds to the metal chalcogenide.[22] Currently, this chemical could be regarded as a mixture of CdS and phosphate. However, describing the CdS-PO surface modifications in terms of a mixture does not accurately describe the type of bonding (e.g. ionic, covalent) taking place on the surface of the CdS nanoparticle.

7.4.6 Description of organics grouping

Nomenclature systems for organic chemicals can be used to describe chemical structure and functionalization. Examples of nano-objects in this grouping include but are not limited to dendrimers, polystyrene and nanocellulose. Nanocellulose, for example, is an organic nano-object which was identified in the ranking exercise. Nanocellulose is extracted from plant, animal, algae and bacterium and is made of cellulose chains packed in a predominantly crystalline structure. Application areas include paper and paperboard, flexible films, composites, food, defence, biomedical, automobile, aerospace, additive manufacturing and oil recovery. Current chemical nomenclature is not useful for capturing the size range of nanocellulose particles embedded in films or differences in optical properties based on particle size. Current chemical nomenclature permits the expression of other molecules and moieties covalently bonded to nanocellulose.

7.4.7 Description of other groupings

There are a plethora of nano-objects which do not fall into the above groupings. Three separate subclasses ranked as being of interest from the survey are endohedral metallofullerenes, nanoclays, and salts (e.g. calcium carbonate nanoparticles). Endohedral metallofullerenes consist of a hollow spherical shell of carbon atoms, about 1 nm in diameter, containing one or several metal atoms inside. Features of interest for chemical nomenclature would include a description of the nature of the metal atom, which contributes to the physical and chemical properties of the material, the carbon shell, and any surface modifications.

Nanoclays consist of clay minerals having a 2:1 expanding crystal lattice. A nominal nanoclay composition might be Al < 10 %, Si > 25 %, H < 5 % and O > 10 % (g/g). Smectite refers to a family of non-metallic clays primarily composed of hydrated sodium calcium aluminium silicate. Powders with particle size in the range of 20 nm are commercially available. Calcium carbonate nanoparticles consist of carbonic acid calcium salt nanoparticles in the range of approximately 10 nm to 80 nm. Desirable properties include cation exchange and plastic properties. Some of the aspects that might be considered for chemical nomenclature development are information related to crystalline structure, solubility features, size, and surface area.

Similar to the discussion for the different groupings above, existing chemical nomenclature for these nano-objects is heavily reliant on describing their molecular connectivity. Features such as surface area, size, and shape, cannot be distinguished by these nomenclature systems.

8 Considerations for a nomenclature system for nano-objects

8.1 General

Fundamentally, it is thought that a naming system to distinguish various nano-objects improves the effectiveness of communication concerning the features, functions and properties of these materials. Given that there are chemical nomenclature systems that are at an advanced stage, which are well-known and commonly used, this Technical Report concludes that an effective approach to developing nomenclature systems for nano-objects would be to start with existing chemical nomenclature frameworks where this is possible.

A fundamental reality facing chemical nomenclature systems with respect to nano-objects is that the emerging nature of the field of nanotechnologies presents challenges in identifying the features essential for identification. Some or all of these features might not be part of existing nomenclature systems. Moreover, care must be taken that proper methods are available to measure these features and to ensure that the latest terminology and scientific information is considered as it becomes available. This Report sets out certain considerations and features that are possibly useful for further development of chemical nomenclature systems for the selected nano-objects listed in Table 1. These suggestions might not be suitable for use in naming all classes of nano-objects, and further deliberation is needed for specific nano-objects. The information presented is intended to provide a rational basis to further explore both the necessity for and approaches to development of nomenclature systems for selected nano-objects.

8.2 General considerations for chemical nomenclature for nano-objects

Chemical nomenclature is a robust system for naming which provides a minimum set of descriptors that enable a knowledgeable person to understand an object's chemical and structural composition. Because of their size, nano-objects could exhibit unique properties not seen in their larger scale counterparts that share the same chemical composition. A nomenclature system designed for naming nano-objects would allow the research community, industry, governments and public interest groups to identify the nano-object in use, distinguish products from others, protect patents, and communicate effectively across a variety of industries and scientific disciplines.

As an initial matter, the following general considerations are offered to assess the degree to which existing chemical nomenclature systems are adequate to provide a common system of naming nano-objects. These considerations are also relevant when developing chemical nomenclature systems for selected nano-objects where such systems either do not exist or are insufficient:

a) the system should be able to describe and distinguish among nano-objects to a reasonable degree;

b) the system should have a minimum set of descriptors that result in names from which a knowledgeable person can understand the nano-object's chemical and structural composition;

c) the naming rules should be sufficiently simple and clear to evaluate studies and work on the same nano-object;

d) the system should be robust to encompass advances in nanotechnologies;

e) for a nomenclature system to be robust, techniques to measure the pertinent parameters should be available.

8.3 Features of interest reported through ISO/TC 229 survey mechanism

The survey of TC 229 member bodies sought information concerning features that survey participants consider important to distinguish nano-objects from each other and from bulk chemical substance counterparts. Table 2 presents representative information from the anecdotal survey submissions by TC 229 member bodies for the selected nano-objects that are ranked as of high interest in Table 1.

Table 2 — Description of ISO/TC 229 survey responses for selected nano-objects and their features of interest

Description of nano-object	Features of interest
Metals	
Gold (Au). Often referenced informally as solid or porous gold nanoparticles, nanowires, nanoshells, or nanocomposites that contain Au. CAS RN 7440–57–5	The diversity and complexity in geometry, surface functionality, and physical and biochemical properties. An assortment of adjectives, e.g. nano-particles, spheres, rods, wires, cubes, prisms, stars, eggs, rice, are used to describe the particle morphology.
Silver (Ag). Preparation methods and conditions result in clusters of various sizes, shapes and state of surface stabilization. Includes clusters with a mean diameter in the range 5 nm to 10 nm and clusters with diameters larger than 20 nm to 30 nm. CAS RN 7440–22–4	Surface effects, including surface charge, surface/interface interactions, and surface plasmon resonance. These nano-objects are distinguished by their shape, size and size distribution, surface chemistry and bonding. Descriptions for core-shell plasmonic nanoparticles and composite plasmonic nanostructures (bi- or tri-metallic alloys).
Metal oxides	
Silicon dioxide (SiO_2). Precipitated silica with size range from 5 nm to 100 nm. CAS RN 7631–86–9 CAS RN 112945–52–5 CAS RN 14808–60–7	Surface effects, including surface charge, surface area, surface/interface interactions. These nano-objects are distinguished by their shape, size and size distribution, surface chemistry and bonding.
Iron oxide (hematite and magnetite) (Fe2O3 and Fe3O4, respectively). The nano-object consists of a spherical core of hematite/magnetite. CAS RN 1309–37–1 CAS RN 1317–61–9	Surface effects, including surface charge, surface area, surface/interface interactions. These nano-objects are distinguished by their shape, size and size distribution, surface chemistry and bonding.
Titanium dioxide (TiO_2). Exists in three phases: anatase, rutile and brookite. Anatase and brookite are stable at low temperatures and the anatase phase completely transforms to the rutile phase at the temperatures around 750° - 900°C. The structural properties and the particle sizes depend on the engineering/ manufacturing processes. Brookite phase CAS RN 13463–67–7 Anatase phase CAS RN 1317–70–0 Rutile phase CAS RN 1317–80–2	Current nomenclature systems do not distinguish the crystalline and the molecular structures of nanoscale TiO_2 from those of the larger scale counterparts. An appropriate nomenclature for nanoparticles might differentiate the structural and chemical characteristics of different nanoscaled TiO_2 in terms of information related to space dimensions (size, shape, etc.) and information related to interactions, for example, core-shell interactions are important in the anatase/rutile phase of TiO_2.
Cerium oxide (CeO_2). Typically consists of nanoparticles ranging from 10 nm to 200 nm. CAS RN 1306–38–3	Surface effects, including surface charge, surface area, surface/interface interactions. These nano-objects are distinguished by their shape, size and size distribution, surface chemistry and bonding.
Carbon	

Table 2 *(continued)*

Description of nano-object	Features of interest
CNTs are tubular members of the graphene structural family; the ends of a nanotube are sometimes capped with a hemisphere of a fullerene-like structure. Their name is derived from their diameter, which is typically on the order of a few nanometers. The CNT family includes SWCNT, MWCNT, DWCNT, and cup-stack carbon nanotube (CSCNT). It also includes derivatives of CNTs (functionalized CNT) and encapsulation compounds of CNTs. CAS RN: 308068–56–6	This class of materials can be manufactured using several different types of chemical processes, under varying process conditions with many different reactants, catalysts or other starting materials. Most SWCNT have a diameter of close to 1 nanometer, with a tube length that can be several orders of magnitude longer. A SWCNT consists of a seamless hollow cylinder with a wall that is composed entirely of a single atomic layer of carbon atoms covalently bonded with sp2 hybridization, a cross-sectional diameter typically in the range of 0,5 nm to 2,5 nm, and ends that are typically capped with hemispherical fullerene-like structure.[23] MWCNTs can be classified by the outer and inner diameters and the number of walls. The bonding of a nanotube is described by applied quantum chemistry, specifically, orbital hybridization. The chemical bonding of nanotubes is composed entirely of sp2 bonds, similar to those of graphite. This bonding structure, which is stronger than the sp3 bonds found in diamonds, provides the molecules with their unique strength. The aspect ratio of these nano-objects may be related to the toxicity features. Chirality is another distinguishing feature.
Nanodiamond. A typical elemental composition of detonation nanodiamond includes about 90 % (g/g) carbon, 5 % to 10 % oxygen, 1 % to 3 % nitrogen and about 1 % hydrogen. Commercial samples may contain also up to 5 % iron and up to 5 % of inert impurities, such as SiO_2 or TiO_2. Diamond 7782–40–3 C_n carbon(*cF*8)	Diamond crystallite (“core”, *sp3* hybridized carbon atoms) coated by a single- or multilayer, fullerene-like, partially oxidized graphene shell (*sp2* hybridized carbon). A transition layer of *sp3*/*sp2* hybridized carbon could form between the core and the shell. Commercially available forms are colloidal sols and readily dispersible powder (agglomerated).[24] Properties of nanodiamond depend on the thickness of carbon shell, graphitization level, particle agglomeration level, the crystalline structure of diamond core, the carbon shell structure, differentiation of particle size, and aggregate size.
Endohedral metalofullerenes	
The nano-object consists of a hollow spherical shell of carbon atoms, about 1 nm in diameter, containing one or several metal atoms inside.[25] IUPAC: [n]fullerene-incar-[m]metal, n = 60, 70, 72, 74, 76, 78, 80, 82, 84, 86, 88, 90; m = 1, 2, 3, 4; metal = Sc, Y, La or lanthanide. MDL number MFCD00133992 (carbon) or MFCD00282904 (fullerenes)	A description of the nature of the metal atom in endohedral metallofullerene, which contributes to the physical and chemical properties of the material.
Organics	
The nano-object consists of rod-like, highly crystalline particles. The surface chains are composed of cellulose for which some hydroxyl groups are substituted during the production process. The typical width can be from 3 nm to 70 nm, and the length can be from 25 nm to 3 000 nm Cellulose sulfate CAS RN 9032–43–3 $(C_6 O_5 H_{10})_{22–28} SO_3H$	Nanocrystalline cellulose (NCC) differs from other cellulose-based materials in regard to its physical properties and surface chemistry and degree of crystallinity.

8.4 Further identification and discussion of key features of nano-objects

8.4.1 General

Certain features are identified in the following sections to illustrate how existing chemical nomenclature could be adapted, while recognizing limitations associated with measuring some of these parameters and/or lack of standardization in measurement methods.[3)]

8.4.2 "Core" particle composition

It is suggested that a system of naming begin by considering the chemical information and crystal structure of the nano-object including chemical composition, presence or absence of crystalline structure including lattice parameters and space group, and impurities, if any. This is a recommended feature for naming a discrete nano-object and each nanoscale region having an interface within the nano-object.

8.4.3 Surface chemistry

An appropriate descriptor for surface chemistry should be considered including composition of the outermost surface and the chemical species attached to that surface.

8.4.4 Particle size

An appropriate descriptor of particle size for consideration is the physical dimensions of a particle determined by specified measurement conditions.

8.4.5 Particle shape

A geometric description of the extremities of the nano-objects or collection of nano-objects, aggregates, agglomerates that make up the material under investigation could be considered. Three ISO categories developed for this purpose are sphere, fibre and plate. Additional descriptors could be needed.

8.5 Illustrations of possible chemical nomenclature approaches for selected nano-objects

More traditionally, chemical nomenclature involves the use of specific molecular structure descriptors in association with chemical composition. Typically, the use of physical/structural parameters has been the exception rather than the rule. Nevertheless, use of one or more of a short set of parameters such as those listed above might be sufficient to distinguish one nano-object from another and reduce ambiguities in the identification of nano-objects. An example of a format that could be used is as follows:

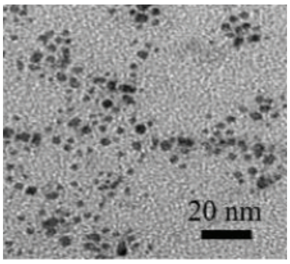
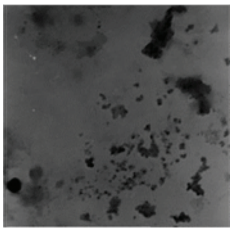
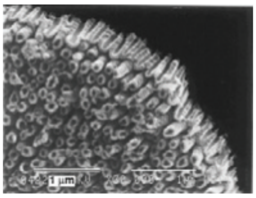
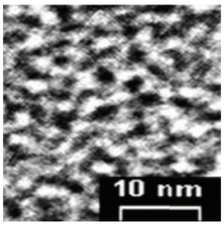
> "Particle Composition-NM; surface functionalization; size; length distribution (if applicable); shape; crystal structure (if known)

This example above uses key parameters in a specific order together with existing chemical nomenclature for identification. The approach can be useful in naming nano-objects in the metal oxides group. To illustrate the approach examples of names for several nanoscale titanium dioxide materials, a well-studied class of nano-objects, are provided which use these parameters in combination with the more conventional name. It is noted that the parameters illustrated in Table 3 are based on their availability in the literature. No effort has been made at this point to determine the appropriateness of particular size ranges or length distributions for differentiating between nano-objects. There is no attempt to

3) For additional reference, there are several sources of information on physical-chemical properties thought to be relevant to describing nanomaterials. These include 1) U.S. Environmental Protection Agency (USEPA). Parameters for Reporting Carbon Nanotubes; [26] 2) Environment Directorate. Joint Meeting Of The Chemicals Committee and The Working Party on Chemicals, Pesticides And Biotechnology. Organisation for Economic Co-Operation and Development. Series on the Safety of Manufactured Nanomaterials No. 27. List of Manufactured Nanomaterials and List of Endpoints for Phase One of the Sponsorship Programme for the Testing of Manufactured Nanomaterials: Revision. ENV/JM/MONO(2010)46; [27] and 3) ISO/TR 13014, Guidance on physico-chemical characterization of engineered nanoscale materials for toxicologic assessment (2012). [28]

imply that titanium dioxide in or outside of the illustrated ranges and distributions results in a uniquely identified new chemical substance.

Table 3 — Sample and illustrative nomenclature parameters for titanium dioxide[29-32]

	Sample description	Illustrative nomenclature
	Titanium dioxide, 2 nm to 5 nm, functionalized with hydroxyl, water, and carbon; anatase; unavailable information on degree of hydration.	Titanium dioxide-NM *(hydration undefined)*; hydroxyl, water and carbon surface functionalization; 2 nm to 5 nm nanoparticle; anatase.
	Titanium dioxide, 3 nm to 8 nm, functionalized with hydroxyl, water and polyethylene glycol, unavailable information on degree of hydration, shape and crystal structure.	Titanium dioxide-NM *(hydration undefined)*; hydroxyl, water and polyethylene glycol surface functionalization; 3 nm to 8 nm; *(shape undefined)*; *(crystalline structure undefined)*.
	Titanium dioxide, hydrated, nanotubes with 70 nm to 100 nm hollow core; 30 nm to 50 nm wall thickness; 140 nm to 180 nm external diameter and 8 µm length; amorphous; unavailable information on surface functionalization.	Titanium dioxide-NM hydrate; *(surface functionalization undefined)*; nanotube; 70 nm to 100 nm hollow core; 30 nm to 50 nm wall thickness; 140 nm to 180 nm external diameter; 8 000 nm length; amorphous.
	Titanium dioxide, surface modified with dodecylbenzenesulfonic acid, 2 nm to 6 nm nanoparticle, rutile structure, and unavailable information on degree of hydration.	Titanium dioxide-NM *(hydration undefined)* dodecylbenzenesulfonic acid surface functionalization; 2 nm to 6 nm nanoparticle; rutile.

Although preliminary, the examples in Table 3 serve to effectively demonstrate how a nomenclature system based on molecular structure could be adapted to distinguish nano-objects through the supplemental use of standardized physical, chemical, or process parameters. The number of undefined parameters in Table 3 also effectively illustrates the need to develop standard parameters associated with established measurement methods.

Other approaches might be more appropriate for other classes of nano-objects. An example of an entirely different method is illustrated by a quantum dot with a II-VI nanocrystalline semiconductor core, a protective shell of another semiconductor composed of another II-VI (or alternatively a III-V semiconductor), and a second shell of a passivating material. These features of the quantum dot are considered important, based on current knowledge, to distinguish it from other quantum dots. In addition, one could arguably consider information such as the shape, dimensions, and crystallographic properties of the core, shell and surface modification.

8.6 Supplemental features of a chemical nomenclature system for nano-objects

8.6.1 General

In addition to establishing a standardized set of rules for naming chemical substances, chemical nomenclature systems can have supplemental features associated with them to facilitate the exchange of information, such as trivial names, randomly generated index numbers, or more complex reference systems that offer links to additional information on the nano-object beyond the name, also called "smart numbering".

CAS provides an arbitrary but unambiguous numeric registry number to identify and list chemical substances. However, additional utility is provided when a system of reference (numeric or alpha-numeric) is organized and administered to offer information on key material properties that can be associated with a chemical substance. An example of a system that associates a reference number with supplemental information is the designator-description nomenclature in use for food dyes (Red Dye No. 2, Blue Dye X, etc.). In this case a simple designator pointing to a detailed description of the specific chemical substance and percentage composition of the dyes is used. Such a system presents advantages in the event that chemical nomenclature threatens to become overly complex in its description.

Another example of such a system can be found in metallurgical nomenclature, in which simple numbers are typical for describing steels, aluminium alloys, copper alloys, with various properties. Examples are the 100, 200, 300, and 400 steels, with "300 steels" generally being the stainless or corrosion resistant steels; 400 steels are stainless with additional feature of being nonmagnetic, etc. In each of these instances the number or designator is a pointer to well-known and established (standardized) descriptions of the elements or compounds and their percentage content in the alloy.

At a minimum then, a simple numbering system could provide a means for both technical and non-technical individuals to identify nano-objects. The numbering might be arbitrarily generated and independent of the nano-object structure, similar to the CAS numbering system. Such a system is also practical for tracking databases and internet searching. A smart numbering system linked to select features/parameters of the nano-object name could prove resource intensive but useful to further understanding of the nano-object.

The following review of numbering systems is offered to describe jurisdiction-specific chemical identification numbers, database registration chemical identifiers, and structure specific chemical identifiers.

8.6.2 EC number

An example of a jurisdiction-specific chemical identification number is the European Commission (EC) number, which is a seven-digit code that is assigned to chemical substances that are commercially available within the European Union. The number is assigned by the Commission of the European Communities and is the official number of a substance in the EU. EC number is made up of seven digits according to the pattern xxx-xxx-x. It can be written in a general form as NNN-NNN-R where R is a check digit and N represents integers.

Example

Name: Formaldehyde

EC number: 200-001-8

8.6.3 Database chemical registration identifiers

These systems link specific compounds to numerical identifiers within specific databases. These numbers are randomly generated and do not contain any structural intelligence.

Example

Name: Formaldehyde

ChemSpider: 692

Beilstein Registry Number; BRN: 1209228

PubChem: 712

Unique Ingredient Identifier; UNII: 1HG84L3525

Chemical Abstracts Service; CAS RN: 50-00-0

8.6.4 SMILES

An example of a structurally descriptive system is the Simplified Molecular Input Line Entry Specification (SMILES) system. SMILES is a specification for unambiguously describing the structure of chemical molecules using ASCII string. An important advantage to this approach is that most molecule editors can convert the strings into either 2D drawings or 3D models of the molecules. SMILES provides information on atoms, bonds, aromaticity, branching, stereochemistry as well as isotopes. It is also quite compact while still being able to represent chemical information.

Example

Name: Formaldehyde

SMILES: C = O

8.6.5 The International Chemical Identifier (InChI)

The International Chemical Identifier (InChI) maintained by IUPAC is a textual identifier for chemical substances. It was developed by IUPAC and the National Institute of Standards and Technology (NIST) during 2000-2005. The identifier describes a chemical substance by layers of information. It includes atoms and their bond connectivity, tautomeric information, isotope information, stereochemistry and electron charge information. InChls differ from CAS registry numbers in three respects. They are freely usable and non-proprietary, can be computed from structural information, and are not assigned by an organization. Most information can be seen at a glance.

Sometimes an InChIKey is used and is a hashed version of InChI. Specifically, it is a fixed length of 25 characters and is a condensed digital representation of the InChI. The InChIKey is designed to allow for easy web searches of chemical compounds.

Example

Name: Formaldehyde

InChI: 1/CH2O/c1-2/h1H2

InChI key: WSFSSNUMVMOOMR-UHFFFAOYAT

8.6.6 Gentleman and Chan

The proposed *Codification of Nanomaterials* by Gentleman and Chan includes a structure-based identification system that encodes the overall composition, size, shape, core and ligand chemistry, and solubility of nanostructures. The system is similar to InChI because it provides a typographic string of minimalist field codes that will facilitate digital archiving as well as searching for desired properties.

Example

Description: 4-nm diameter CdSe NC capped with PAMAM dendrimer

Codification: 2D-4H-(Cd, Se)-[(Amn, Amn)]-O

8.6.7 Thomas et al.

The numerical system offered by Thomas et al. provides a structure- and formulation-based scheme that identifies the composition of both the nanoparticles and the overall formulation in which they are found. The system has similarities to the nomenclature of Gentleman and Chan but offers a general and extensible framework – at the expense of additional complexity – to provide a more complete description of a nanoparticle formulation.

9 Coordination and timing

Established nomenclature systems are not structured to incorporate size in their naming conventions. This has led to current ambiguities, inconsistencies and inaccuracies in the naming and identification of nano-objects. This Technical Report has examined chemistry-based nomenclature systems for possible adaption to include additional descriptive parameters to assign names to nano-objects.

Systems of chemical nomenclature tend to lag behind technology developments. Nomenclature development typically occurs when there is a significant body of knowledge about the chemistry and when aspects are meaningful for the purpose of naming. For this reason, certain classes of nano-objects discussed in this Technical Report were assessed for their readiness in developing chemical nomenclature systems. Carbon nanotubes, in particular, appear in need of a common naming system in light of the complete absence of a harmonized chemical nomenclature approach for this class of nano-objects currently. Due to the level of complexity in distinguishing among CNTs, it is expected that this body of work could take a number of years, but that sufficient knowledge exists currently to begin this work. At the same time, consideration could be given to nomenclature for well-characterized nano-objects such as gold nanoparticles, a comparatively less complex task from a nomenclature perspective.

There are a number of challenges and hurdles to be overcome when developing a chemical nomenclature system for nano-objects. The development, implementation and acceptance of a chemical nomenclature for nano-objects will take a number of years. It is expected that ISO/TC 229/JWG 1 has a valuable role to play in providing coordination, expertise, planning and resources associated with projects of this magnitude.

One of the goals of administering chemical nomenclature for nano-objects is to harness limited resources and the highly specialized expertise that is needed to develop chemical nomenclature for specific nano-object subclasses. Furthermore, such an effort ultimately requires a means of placing the outcome of this work (i.e. nomenclature systems) into the public domain. It is expected that public release of nano-object nomenclature specifications would originate from IUPAC through collaboration with ISO/TC 229/JWG 1. In September, 2009, a formal Category A liaison was established between JWG1 and IUPAC in the field of terminology and nomenclature for nanotechnologies. This liaison permits collaboration on terminology and nomenclature and together, the two organizations can share expertise and experience. It is anticipated that the development of chemical nomenclature specific to nano-objects will proceed in cooperation with IUPAC experts, with the understanding that TC 229 could identify near-term or longer-term course corrections as experience is gained in developing and deploying such systems.

Annex A
(informative)

General nomenclature systems

See Table A.1.

Table A.1 — General nomenclature systems

Name	Summary of Nomenclature System	Comments
CHEMICAL ABSTRACTS SYSTEM (CAS) OF POLYMER NOMENCLATURE Reference: "Naming and Indexing of Chemical Substances for CHEMICAL ABSTRACTS." *A reprint of Appendix IV from the CHEMICAL ABSTRACTS 1987 Index Guide*.[33]	The approach indicates the polymer's starting monomers and reactants in the following general format: Monomer A, polymer with monomer B, monomer C and Monomer D Typically, the most reactive monomer is listed first (e.g. 2-Propenoic acid, 2-methyl-). The first monomer name is followed by a statement "polymer with" (e.g. 2-Propenoic acid, 2-methyl-, polymer with). The remaining monomers are then listed; reactants or counter ions are typically listed last. (e.g. 2-Propenoic acid, 2-methyl-, polymer with butyl 2-propenoate, ethenylbenzene and 2-hydroxyethyl 2-methyl-2-propenoate, compd. with 1,1'-iminobis[2-propanol]).	The system described is based on monomers and reactants without requiring information on polymeric structure, size, or properties that can vary according to size or constituents. This might be useful in the case where structures for some nano-objects are unknown and/or vary substantially.
NOMENCLATURE RULES AND GUIDELINES FOR DISCRETE (I.E. NON-UVCB) CHEMICALS International Union of Pure and Applied Chemistry (IUPAC) and CAS References: "General Principles of Organic Nomenclature R-1.0 INTRODUCTION." *R-1.0 INTRODUCTION*. Advanced Chemistry Development, Inc., n.d. Web. 23 Aug. 2012. < http://www.acdlabs.com/iupac/nomenclature/93/r93_125.htm>.[34] "Recommendations 1993." *Recommendations 1993.* Blackwell Scientific Publications, 1993. Web. 23 Aug. 2012. < http://www.acdlabs.com/iupac/nomenclature/93/r93_15.htm>.[35] "Naming and Indexing of Chemical Substances for CHEMICAL ABSTRACTS." *A reprint of Appendix IV from the CHEMICAL ABSTRACTS 1987 Index Guide*.[33]	The name of a discrete chemical includes parent structure, substituents, and location of substituents on the parent structure. • Parent Structure The parent structure is generally named by identifying the longest constituent of the chemical structure. Substituents Substituents are defined as any chemical groups added to the parent structure and are named according to its chemical class (e.g. alcohol with a 5 carbon chain is called pentanol where an "ol" is added to the end of the name). The substituents are either added as a prefix (beginning of the parent structure) or as a suffix (end of parent structure). The suffix is typically the most senior chemical group, as ranked in a list used by CAS and IUPAC (e.g. for acids, peroxy acids are ranked higher then carboxylic acids). Locants – relative numbering of substituents: Numbering is very important to identify unambiguously chemicals of similar structure. Typically, an organic chemical is numbered starting from one end of the structure or from a substituent. For example, the following chemical is named as cyclohexan-1-one, where the ring is numbered starting from the carbon containing the oxygen as 1. If there is more than one substituent, the numbers are assigned beginning at a designated substituent.	Nano-object nomenclature would likely benefit from the use of a parent structure or a core as the foundation of the name. The system is ideal for a discrete chemical with a well-understood structure. Locant nomenclature might not be directly relevant in cases such as fullerenes and dendrimers. Additionally, CAS and IUPAC have nomenclature conventions for inorganic chemical substances, and substances of Unknown or Variable composition, Complex reaction products or Biological materials. These conventions will have relevance for nanomaterials that are inorganic or complex, including hybrid materials

Table A.1 *(continued)*

Name	Summary of Nomenclature System	Comments
INTERNATIONAL TABLES OF THE COMMISSION ON CRYSTALLOGRAPHIC NOMENCLATURE OR THE ONLINE DICTIONARY OF CRYSTALLOGRAPHY Commission on Crystallographic Nomenclature References: Main Page Crystallography. *Online Dictionary of Crystallography*. N.p., 23 Jan. 2012. Web. 23 Aug. 2012. http://reference.iucr.org/dictionary/Main_Page[36] General Information. International Union of Crystallography. 21 Oct. 2002. Web. 23 Aug. 2012. < http://ww1.iucr.org/comm/cnom/index.html>.[37]	Names stem from geometric shapes, symmetry patterns, and alphanumeric combinations that represent characteristics of a crystal. <u>Crystal Families (Systems)</u> Crystals belong to the same crystal family if they have the same type of conventional cell, regardless of the presence or absence of centering nodes. For example, an orthorhombic crystal with primitive lattice and an orthorhombic crystal with face-centred lattice belong to the same crystal family (*orthorhombic*). <u>Crystal Classes</u> There are two variations of crystal classes, arithmetic and geometric classes. Geometric classes classify symmetry groups of the external shape of macroscopic crystals, namely according to the morphological symmetry. Arithmetic crystal classes are obtained in an elementary fashion by combining the geometric crystal classes and the corresponding types of Bravais lattices (arrangements of ions and particles). For example, in the monoclinic system, there are three geometric crystal classes – 2, m and 2/m – and two types of Bravais lattices – P and C. There are therefore six monoclinic arithmetic crystal classes. Their symbols are obtained by juxtaposing the symbol of the geometric class and that of the Bravais lattice, in that order: 2P, 2C, mP, mC, 2/mP, 2/mC.	This is an efficient naming system based upon geometric shape and symmetry. However, non-experts could have a difficult time discerning the meaning of names without knowing the symbols or which classes belong to which system. This system needs to be more fully examined for its ability to properly describe the crystalline structures of nano-objects.
PROCEDURES AND GUIDELINES ON MINERAL NOMENCLATURE Commission on New Minerals and Mineral Names Reference: Commision on New Minerals, Nomenclature and Classification. International Mineralogical Association. IMA-CNMNC, n.d. Web. 24 Aug. 2012. < http://pubsites.uws.edu.au/ima-cnmnc/ >[38]	Names are based upon well-defined chemical composition and crystallographic properties. Properties traditionally reported for mineral classification include colour, hardness, optical properties, etc. For example, *Hydroxylapatite* and *fluorapatite* both crystallize in the hexagonal crystal system, with the same space group, and have similar unit-cell parameters. They are different species of mineral, however, because the relevant structural site is predominantly occupied by OH in hydroxylapatite and by F in fluorapatite. *Graphite* and *diamond* are allotropes of crystalline carbon; both have the same composition but their structures are different, and therefore minerals such as these are regarded as separate species. Names might also include a reference to geographical locality of occurrence, discoverer of the mineral, a person prominent in the field, or a particular property of the mineral. Future guidelines may consider how size affects mineral classification.	This nomenclature might not be relevant to many organic or amorphous materials. For experts, the names assigned by this system to relevant substances deliver a basic understanding of individual composition and structure. Non-experts will not necessarily understand how the name relates to composition or structure. There is a degree of lack of uniformity, as mineral classification for complex forms are considered on a case-by-case basis.

Table A.1 *(continued)*

Name	Summary of Nomenclature System	Comments
INTERNATIONAL UNION OF BIOCHEMISTRY AND MOLECULAR BIOLOGY (IUBMB) NOMENCLATURE FOR NAMING OF ENZYMES References: Classification and Nomenclature of Enzymes by the Reactions They Catalyse. *Enzyme Classification*. Nomenclature Committee of the International Union of Biochemistry and Molecular Biology. Web. 23 Aug. 2012. < http://www.chem.qmul.ac.uk/iubmb/enzyme/rules.html>[39] EC 1.1.1.1 - Alcohol Dehydrogenase. *EC 1.1.1.1 - Alcohol Dehydrogenase*. N.p., n.d. Web. 23 Aug. 2012. < http://www.brenda-enzymes.info/php/result_flat.php4?ecno=1.1.1.1>.[40]	For enzymes, there are 3 overarching rules for naming and issuing corresponding registry code numbers. First, enzyme names typically end with the suffix –*ase.* Second, enzymes are named according to the reaction they catalyse. The chemical reaction catalysed is the specific property that distinguishes one enzyme from another. For example, the enzyme that catalyses an aldehyde dehydrogenation reaction is referred to as aldehyde dehydrogenase. Third, enzymes are further divided on the basis of their target substrate. For example, an alcohol dehydrogenase is further categorized to gastric alcohol dehydrogenase, octanol dehydrogenase, retinol dehydrogenase, etc. <u>Registry Numbers</u> Enzymes are given a registry number on the basis of the type of reaction they catalyse. The numbering system follows a tree hierarchy starting from the general type of reaction to more specific reactions. This numbering system provides additional information such as physical-chemical properties, inhibitors, stability, application, etc. For example, - alcohol dehydrogenase is given the registry number 1.1.1.1 where: 1. refers to the general oxidoreductases; 1.1 refers to acting on the CH-OH group of donors; 1.1.1 with NAD+ or NADP+ as acceptor; and 1.1.1.1 to the specific alcohol dehydrogenase reaction system.	This system allows for the use of a trivial name, without having to resort to a long systematic name, while having the same link via a registry number to information that the systematic name provides. Names include more than one parameter, but do not contain chemical or structural information. Instead, information is based on the target substrate.
INTERNATIONAL CODE OF VIRUS CLASSIFICATION AND NOMENCLATURE International Committee on Taxonomy of Viruses References: THE INTERNATIONAL CODE OF VIRUS CLASSIFICATION AND NOMENCLATURE. *International Committee on Taxonomy of Viruses*. ICTV, 2012. Web. 24 Aug. 2012. < http://www.ictvonline.org/codeOfVirusClassification_2002.asp?bhcp=1 >.[41]	ICTV maintains an index of viral names. The naming code employs the use of hierarchical levels of Order, Family, Subfamily, Genus, and Species and places responsibility for serotypes, genotypes, strains, variants and isolates of virus species on acknowledged international specialist groups. The name of a discrete viral taxon should reflect viral evolutionary relationships and individual phylogenies. For example, *audovirales* and *Mononegavirales* are names for two different order of virus, each name standing for different descriptors. *Caudovirales* is an order of virus categorized by tailed baceteriophages, while *Mononegavirales* is an order of viruses categorized by a non-segmented, negative sense RNA genome.	Names derived with this system provide predictability and for experts, deliver a basic understanding of individual viral phylogenies. Certain names require input from specialists; non-experts might not understand how the name relates to characteristics of the virus or phage.
GLOBAL MEDICAL DEVICE NOMENCLATURE Global Medical Device Nomenclature Agency References: GMDN Home Page. Global Medical Device Nomenclature Agency, 2011. Web. 23 Aug. 2012. < http://www.gmdnagency.com/?id=nom>.[42] Patient Safety, Quality and Risk Management. *Universal Medical Device Nomenclature Systemâ„¢*. ECRI Institute, 2012. Web. 23 Aug. 2012. < https://www.ecri.org/Products/Pages/UMDNS.aspx>.[43]	This system consists of a list of coded descriptors to generically identify medical devices and related health care products together with a numerical identifier. Names are based upon a three-tiered system for classifying medical devices. Names consist of categories, template terms (which are broad names that group similar preferred terms), and preferred terms (which are names for devices that have the same or similar intended purpose). EXAMPLE 10035 – Adhesive, aerosol, general purpose and 10126 – alarm, blood-pressure describe two different medical devices, which can be identified based upon the GMDN number or the names alone.	The system appears efficient in grouping devices into categories. The numbering system allows experts and non-experts the ability to locate a particular device. Some devices could fit one or more categories; non-experts might not have the ability or the knowledge to group medical devices themselves. Indexing by an identifiable number is a tool for attempting an unambiguous naming system. Nanoscale devices might be incorporated in this system in the future.

Annex B
(informative)

Selected nano-object-specific nomenclature systems

B.1 Nomenclature for fullerenes (IUPAC)

B.1.1 Reference

"NOMENCLATURE AND TERMINOLOGY OF FULLERENES: A PRELIMINARY SURVEY." *Pure and Appl. Chem.* 69 1997: 1411-434.[44]

B.1.2 Brief description of system (e.g. descriptors)

a) Fullerene or *quasi*-fullerene

b) The number of carbons in the molecule

c) The point group symmetry (I_h, C_{2v}, etc.)

d) Additional Roman numbers to subdivide fullerenes with the same point-group symmetry (I, II, III, ...)

e) The types of constituent rings in parentheses in the case of *quasi*-fullerene

NOTE This nomenclature system is different from the corresponding CAS system.

EXAMPLE

	IUPAC	**CAS**
C_{60}	[60-I_h]fullerene	[5,6]fullerene-C_{60}-I_h
C_{78}	[78-C_{2v}(I)]fullerene	[5,6]fullerene-C_{78}-C_{2v}
C_{48}	(4,6,8)[48-O_h]*quasi*-fullerene	[4,6,8]fullerene-C_{48}-O_h

The point group symmetry is a good descriptor for fullerene structures.

There can be many fullerene isomers with the same point-group symmetry, and the additional Roman numbers are introduced to distinguish them, but the rule for this numbering is not easy, especially for large fullerenes with low symmetry.

B.1.3 Relevant aspects and/or descriptors for a nomenclature system for nano-objects

Adding some characters before and/or after the basic name of a nano-object (in this case, "fullerene") is a good practice, which can be applicable to nano-objects.

B.2 Nomenclature for carbon black used in rubber products (ASTM International)

B.2.1 Reference

ASTM D1765-10. *Standard Classification System for Carbon Blacks Used in Rubber Products*. ASTM International. 23 Aug. 2012. < http://www.astm.org/Standards/D1765.htm>.[45]

B.2.2 Brief description of system (e.g. descriptors)

Scope: This system covers the classification of rubber-grade carbon blacks by the use of a four-character nomenclature system. The first character gives some indication of the influence of the carbon black on the rate of cure of a typical rubber compound containing the black. The second character gives information on the average surface area of the carbon black. The last two characters are assigned arbitrarily.

The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

B.2.3 Relevant aspects and/or descriptors for a nomenclature system for nano-objects

This type of nomenclature is useful for a specific material used for a specific application. However, it might be too complex to introduce this type of authorized registration system for the entire universe of nano-objects. A multi-digit coding system based on several descriptors might be possible for nano-objects, if a tree-like classification system, such as the “nano-tree”, is used.

Annex C
(informative)

Selected public listings of nano-objects

C.1 ISO/TC 229 nano-objects identified in program of work

SWCNT	nano-calcium carbonate
MWCNT	nano-titanium dioxide
metal nanoparticles	

C.2 OECD WPMN list of representative manufactured nanomaterials in the test programme (year 2012)

fullerenes	cerium oxide
SWCNT	nanoclays
MWCNT	iron nanoparticles
silver nanoparticles	silicon dioxide/silica
gold nanoparticles	dendrimers
titanium dioxide	zinc oxide
aluminium oxide	

C.3 NICNAS priority nanomaterials for risk assessment

titanium dioxide	fullerenes
zinc oxide	CNTs
cerium oxide	nanosilver

C.4 REFNANO priority 1 candidate materials for toxicology

Material	Comments
Carbon black	available in nano and micro-sizes; already well-studied in humans and animals providing a good starting point.
• TiO_2	available in nano and micro-sizes, and in coated and uncoated forms; already well studied in humans and animals providing a good starting point.
• ZnO	• available in coated and uncoated forms.
• SWCNT and MWCNT	• straight rigid forms should be available along with bundled forms; long and short lengths should be available.
• Polystyrene (Fluorescent)	available with different surface modifications in any one size; should be available in forms for tracking fate in cells; should be available in a range of different sizes in the nanometre scale.
• Ag	• Ag has increasing use for antibacterial properties including disinfectant sprays and wound dressings.

Material	Comments
• Other key metals and metal oxides	• Priorities for ecotoxicology: Zn, Cu, Ni, Fe and their oxides.
• Combustion derived NP	• To be used as a control particle since there is already a significant body of literature, risk and toxicology information available.

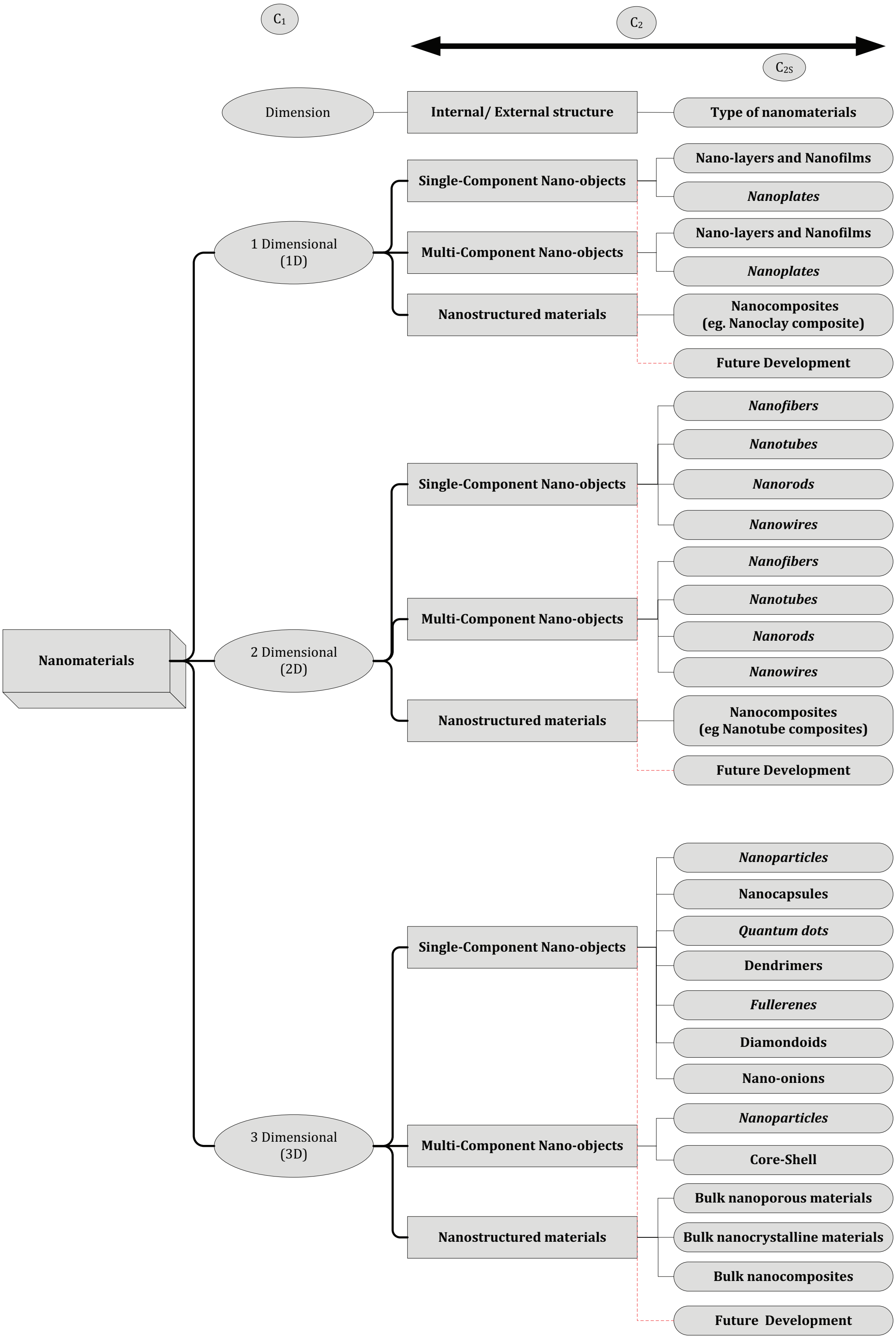
C.5 US. Nanoscale Materials Stewardship Program

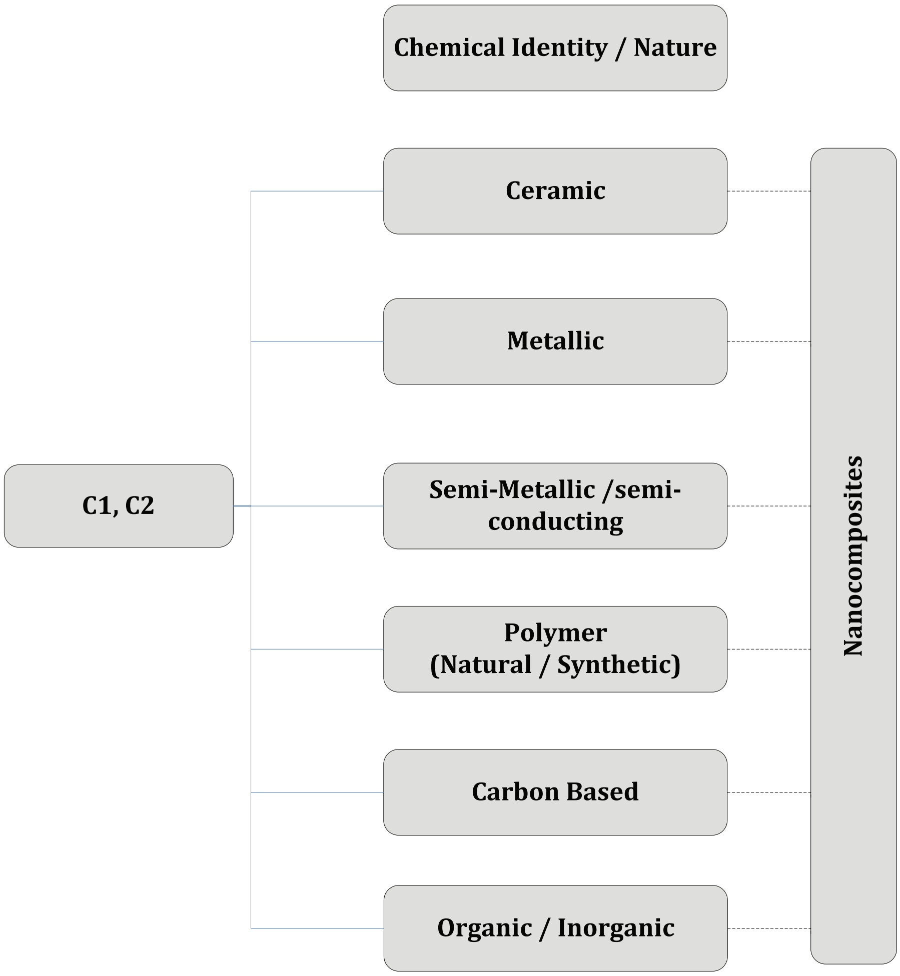
aluminium oxide	manganese oxide
antimony pentoxide	MWCNT
calcium oxide	nanoclays
carbon black	nickel nanoparticles
cerium oxide	palladium nanoparticles
cluster diamonds	platinum nanoparticle
cobalt nanoparticles	rhodium nanoparticles
copper oxide	silicates
fullerenes	silicon dioxide/silica
gold nanoparticles	silver nanoparticles
iron oxide	SWCNT
iron cobalt	titanium dioxide
lithium titanate	titanium oxide
magnesium oxide	zinc oxide

C.6 California Department of Toxic Substances Control

quantum dots	nano-silver
nano-titanium dioxide	nano-zerovalent iron
nano zinc oxide	

C.7 Select components of ISO/TR 11360[5]




Chemical Identity / Nature
C1, C2
Ceramic
Metallic
Semi-Metallic /semi-conducting
Polymer (Natural / Synthetic)
Carbon Based
Organic / Inorganic
Nanocomposites

C.8 Nanomaterials commercially available on Nanowerk database (as of December 2010)[21]

Class of Material	Name of material	# of Suppliers
MWCNT	Carbon (Carbon Nanotubes (DWNT (functionalised))	3
	Carbon (Carbon Nanotubes (DWNT (pure))	30
	Carbon (Carbon Nanotubes (MWNT (doped))	1
	Carbon (Carbon Nanotubes (MWNT (film))	4
	Carbon (Carbon Nanotubes (MWNT (functionalised))	165
	Carbon (Carbon Nanotubes (MWNT (other))	4
	Carbon (Carbon Nanotubes (MWNT (paper))	1
	Carbon (Carbon Nanotubes (MWNT (pure))	290
	Carbon (Carbon Nanotubes (MWNT (tips))	5
	Total	**503**
SWCNT	Carbon (Carbon Nanotubes (SWNT (film))	1
	Carbon (Carbon Nanotubes (SWNT (functionalised))	42
	Carbon (Carbon Nanotubes (SWNT (gel))	1
	Carbon (Carbon Nanotubes (SWNT (pure))	107
	Total	**151**
Titanium dioxide	Titanium dioxide (Nanoparticles of binary compounds)	3
	Titanium oxide (Nanoparticles of binary compounds)	66
	Titanium oxide (anatase / titanium III oxide) (Nanoparticles of binary compounds)	9
	Total	**78**
Silver nanoparticles	Silver (Nanofibres)	1
	Silver (Nanoparticles of Elements)	77
	Silver (Nanowires)	9
	Total	**87**
Fullerenes	Carbon (Fullerenes (C-13 enriched))	6
	Carbon (Fullerenes (Chemically modified))	50
	Carbon (Fullerenes (Doped film))	4
	Carbon (Fullerenes (Film))	4
	Carbon (Fullerenes (fullarene mixture))	7
	Carbon (Fullerenes (Fullerene soot))	2
	Carbon (Fullerenes (Metal endohedrals))	3
	Carbon (Fullerenes (pure C60 - C84))	49
	Carbon (Fullerenes (Sublimed))	4
	Total	**129**
Silicon dioxide/ silica	Silicon dioxide (Nanoparticles of binary compounds)	1
	Silicon oxide (Nanoparticles of binary compounds)	70
	Total	**71**

Class of Material	Name of material	# of Suppliers
Gold nanoparticles	Gold (Nanoparticles of Elements)	125
	Gold (Nanowires)	1
	Gold/tetra-n-octylammonium chloride (Complex nanomaterials)	1
	Total	**127**
Iron oxide	Iron (“magnetic iron oxide”) (Nanoparticles of Elements)	84
	Iron (II/III) oxide (Nanoparticles of binary compounds)	18
	Iron (III) oxide (Nanoparticles of binary compounds)	6
	Iron oxide (Nanoparticles of binary compounds)	37
	Iron oxide (haematite) (Nanoparticles of binary compounds)	1
	Iron oxide (Maghemite F2O3) (Nanofibres)	1
	Iron oxide (Magnemite) (Nanoparticles of binary compounds)	1
	Total	**148**
Cerium oxide	Cerium oxide (Nanoparticles of binary compounds)	34
	Total	**34**
Copper nanoparticles	Copper (Nanoparticles of Elements)	35
	Copper (Nanowires)	1
	Copper carbon (Complex nanomaterials)	1
	Copper carbon-coated (Complex nanomaterials)	1
	Total	**38**
Zinc oxides	Zinc oxide (Nanoparticles of binary compounds)	53
	Zinc oxide (Nanowires)	1
	Zinc oxide (Al-doped) (Complex nanomaterials)	1
	Zinc oxide (Ga-doped) (Complex nanomaterials)	1
	Total	**56**
Aluminium oxide	Aluminium oxide (Nanofibres)	1
	Aluminium oxide (Nanoparticles of binary compounds)	64
	Aluminium oxide (Boehmite) (Nanoparticles of binary compounds)	1
	Aluminium oxide/ Chromium oxide (Complex nanomaterials)	1
	Total	**67**
Nickle nanoparticles	Nickel (Nanoparticles of Elements)	28
	Nickel carbon (Complex nanomaterials)	1
	Nickel carbon-coated (Complex nanomaterials)	1
	Nickel/tetra-n-octylammonium chloride (Complex nanomaterials)	1
	Total	**31**

Class of Material	Name of material	# of Suppliers
Quantum dots	Quantum Dots - amino (PEG) modified (Quantum Dots - Biomedical)	3
	Protein A Conjugate (Quantum Dots - Biomedical)	7
	Protein G Conjugate (Quantum Dots - Biomedical)	7
	Quantum Dots - carboxyl modified (Quantum Dots - Biomedical)	13
	Rabbit anti-6xHis Conjugate [Whole IgG] (Quantum Dots - Biomedical)	2
	Rabbit anti-Dansyl Conjugate [Whole Monoclonal IgG] (Quantum Dots - Biomedical)	1
	Rabbit anti-Goat IgG Conjugate (Quantum Dots - Biomedical)	1
	Rabbit anti-Goat IgG, H&L Specificity, F(ab\’)2 fragment (Quantum Dots - Biomedical)	7
	Rabbit F(ab\’)2 anti-Goat IgG Conjugate (Quantum Dots - Biomedical)	1
	Rat anti-Dinitrophenol Conjugate [Whole Monoclonal IgG] (Quantum Dots - Biomedical)	1
	Non-functional CdSe/ZnS QDs (Quantum Dots - Biomedical)	7
	Non-functional InGaP/ZnS QDs (Quantum Dots - Biomedical)	2
	Non-targeted QDs (Quantum Dots - Biomedical)	4
	Organic QDs (Quantum Dots - Biomedical)	7
	Mouse anti-Phosphotyrosine Conjugate [Whole Monoclonal IgG] (Quantum Dots - Biomedical)	2
	Antibody Conjugation Kit (Quantum Dots - Biomedical)	6
	Biotin conjugate (Quantum Dots - Biomedical)	9
	Cadmium mercury telluride (Quantum Dots)	1
	Cadmium selenide (Quantum Dots)	27
	Cadmium selenide/Cadmium sulfide (Quantum Dots)	1
	Cadmium selenide/Cadmium sulfide/Zinc sulfide (Quantum Dots)	1
	Cadmium selenide/Zinc sulfide (amino (PEG) modified (Quantum Dots - Biomedical)	7
	Cadmium selenide/Zinc sulfide (carboxyl modified (Quantum Dots - Biomedical)	7
	Cadmium selenide/Zinc sulfide (Quantum Dots)	83
	Cadmium sulfide (Quantum Dots)	7
	Cadmium sulfide (Quantum Dots)	6
	Cadmium sulfide/Selenide/Zinc sulfide (Quantum Dots)	15
	Cadmium sulfide/Zinc sulfide (Quantum Dots)	1
	Cadmium telluride (Quantum Dots)	26
	Cadmium telluride/Cadmium sulfide (Quantum Dots)	3
	Sheep anti-Digoxigenin Conjugate [Fab Fragment] (Quantum Dots - Biomedical)	3
	Streptavidin Conjugate (Quantum Dots - Biomedical)	18
	Cell labelling kits (Quantum Dots - Biomedical)	7
	Goat anti-chicken igY conjugate (Quantum Dots - Biomedical	1
	Goat anti-fluorescein Conjugate [Whole IgG] (Quantum Dots - Biomedical)	3
	Goat anti-glutathione S-transferase conjugate [whole IgG] (Quantum Dots - Biomedical)	2
	Goat anti-Guinea-pig IgG, H and L specificity, F(ab\’)2 fragment (Quantum Dots - Biomedical)	7
	Goat anti-Human IgG, H and L specificity, F(ab\’)2 fragment (Quantum Dots - Biomedical)	7
	Goat anti-Mouse igG conjugate (Quantum Dots - Biomedical)	3
	Goat anti-Mouse IgG, H and L specificity, F(ab\’)2 fragment (Quantum Dots - Biomedical)	7
	Goat anti-Rabbit igG conjugate (Quantum Dots - Biomedical)	3

Class of Material	Name of material	# of Suppliers
Quantum dots (continued)	Goat anti-Rabbit IgG, H and L specificity, F(ab\')2 fragment (Quantum Dots - Biomedical)	7
	Goat anti-Rat igG (Quantum Dots - Biomedical)	2
	Goat anti-Rat IgG, H and L specificity, F(ab\')2 fragment (Quantum Dots - Biomedical)	7
	Goat F(ab\')2 anti-Human IgG Conjugate (Quantum Dots - Biomedical)	3
	Goat F(ab\')2 anti-Mouse IgG Conjugate (Quantum Dots - Biomedical)	11
	Goat F(ab\')2 anti-Rabbit IgG Conjugate (Quantum Dots - Biomedical)	11
	Goat F(ab\')2 anti-Rat IgG Conjugate (Quantum Dots - Biomedical)	3
	Goat Whole IgG anti-Chicken IgY Conjugate (Quantum Dots - Biomedical)	2
	Goat Whole IgG Conjugate anti-Chicken IgY (Quantum Dots - Biomedical)	1
	Indium gallium Phosphide/Zinc sulfide (amine modified (Quantum Dots - Biomedical)	2
	Indium gallium Phosphide/Zinc sulfide (biotin modified (Quantum Dots - Biomedical)	2
	Indium gallium Phosphide/Zinc sulfide (carboxyl modified (Quantum Dots - Biomedical)	2
	Indium gallium Phosphide/Zinc sulfide (Quantum Dots)	2
	Streptavidin Conjugate (Quantum Dots - Biomedical)	18
	Wheat Germ Agglutinin Conjugate (Quantum Dots - Biomedical)	1
	Zinc selenide (Quantum Dots)	2
	Total	**402**
Zirconium oxide	Zirconium oxide (Complex nanomaterials)	1
	Zirconium oxide (Nanoparticles of binary compounds)	33
	Zirconium oxide / Cerium oxide (Complex nanomaterials)	1
	Zirconium oxide, 3 % yttria stabilized (Complex nanomaterials)	1
	Zirconium oxide, 8 % yttria stabilized (Complex nanomaterials)	1
	Zirconium (IV) oxide (Nanoparticles of binary compounds)	1
	Total	**38**
Nano diamond	Carbon (“Nanoparticles of Elements” (nanodiamonds))	20
	Carbon (“Nanoparticles of Elements” (nanodiamond/nanographite mixture))	2
	Total	**22**
Magnesium oxide	Magnesium oxide (Nanoparticles of binary compounds)	**21**
	Total	**21**
Copper oxide	Copper oxide (Nanoparticles of binary compounds)	13
	Copper oxide and samarium doped oxide (Complex nanomaterials)	1
	Copper oxide and yttria stabilized zirconia (Complex nanomaterials)	1
	Total	**15**
Aluminium nanoparticles	Aluminium (Nanoparticles of Elements)	22
	Total	**22**
Silicone carbide	Silicone carbide (Nanoparticles of binary compounds)	21
	Total	**21**

Class of Material	Name of material	# of Suppliers
Cobalt nanoparticles	Cobalt (Nanoparticles of Elements)	16
	Cobalt carbon-coated (Complex nanomaterials)	1
	Total	**17**
Aluminium nitride	Aluminium nitride (Nanoparticles of binary compounds)	12
	Total	**12**
Antimony tin oxide	Antimony tin oxide (Complex nanomaterials)	12
	Total	**12**
Barium titanate	Barium titanate (Complex nanomaterials)	13
	Total	**13**
Cobalt oxide	Cobalt oxide (Nanoparticles of binary compounds)	**15**
	Cobalt/Cobalt oxide (Nanoparticles of binary compounds)	**1**
	Total	**16**
Graphene	Carbon (Graphene (film))	3
	Carbon (Graphene (flakes))	13
	Carbon (Graphene (on substrate))	2
	Carbon (“Nanoparticles of Elements” (nanographite))	4
	Total	**22**
Silicon nanoparticles	Silicon (Nanoparticles of Elements)	12
	Total	**12**
Silicon nitride	Silicon nitride (Nanoparticles of binary compounds)	19
	Silicon Nitride (Nanowires)	1
	Silicon nitride/carbide (Complex nanomaterials)	1
	Total	**21**
Tin oxide	Tin oxide (Nanoparticles of binary compounds)	11
	Total	**11**
Titanium nanoparticles	Titanium (Nanoparticles of Elements)	15
	Total	**15**
Titanium nitride	Titanium nitride (Nanoparticles of binary compounds	15
	Total	**15**
Yttria stabilized zirconia	Yttria stabilized zirconia (Complex nanomaterials)	18
	Total	**18**
Yttrium oxide	Yttrium oxide (Nanoparticles of binary compounds)	13
	Total	**13**

Class of Material	Name of material	# of Suppliers
Zinc nanoparticles	Zinc (Nanoparticles of Elements)	15
	Total	**15**
Indium oxide	Indium oxide (Nanoparticles of binary compounds)	8
	Indium oxide/tin oxide (Complex nanomaterials)	2
	Total	**10**
Antiomy oxide	Antimony oxide (Nanoparticles of binary compounds)	4
	Total	**4**
Iron-Cobalt	Iron cobalt (Complex nanomaterials)	3
	Iron cobalt magnetic fluid (Complex nanomaterials)	2
	Total	**5**
Palladium nanoparticles	Palladium (Nanoparticles of Elements)	3
	Total	**3**
Platinum nanoparticles	Platinum (Nanoparticles of Elements)	7
	Total	**7**
Calcium carbonate	Calcium carbonate (Nanoparticles of binary compounds)	4
	Total	**4**
Lithium titanate	Lithium titanate spinel (Complex nanomaterials)	2
	Total	**2**
Manganese oxide	Manganese oxide (Nanoparticles of binary compounds)	2
	Total	**2**
Calcium oxide	Calcium oxide (Nanoparticles of binary compounds)	1
	Total	**1**

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