

Designation: E3206 - 19

Standard Guide for Reporting the Physical and Chemical Characteristics of a Collection of Nano-Objects¹

This standard is issued under the fixed designation E3206; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope

- 1.1 This guide provides guidelines for a description system to report the physical and chemical characteristics of collections of nano-objects. It establishes information categories and descriptors useful in describing collections of nano-objects uniquely and such that the equivalency of two or more collections of nano-objects can be determined according to specific criteria.
- 1.2 This guide is designed to be directly applicable to reporting the physical and chemical characteristics of collections of nano-objects in most circumstances, including, but not limited to, reporting original research results in the archival literature, developing ontologies, database schemas, data repositories, and data reporting formats, specifying regulations, and enabling commercial activity.
- 1.3 This guide is applicable to collections of naturally occurring, engineered, and manufactured nano-objects.
- 1.4 One goal of the guide is to help ensure that when measurement results are reported, they are reported uniformly.
- 1.5 A second goal of the guide is to encourage reports on the properties and functionalities of a collection of nano-objects to include as much detail as possible about the physical and chemical characteristics of that collection so it is uniquely specified.
- 1.6 This guide does not cover the chemical reactions or reactivity of a collection of nano-objects.
- 1.7 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.
- 1.8 This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the

responsibility of the user of this standard to establish appropriate safety, health, and environmental practices and determine the applicability of regulatory limitations prior to use.

1.9 This international standard was developed in accordance with internationally recognized principles on standardization established in the Decision on Principles for the Development of International Standards, Guides and Recommendations issued by the World Trade Organization Technical Barriers to Trade (TBT) Committee.

2. Referenced Documents

2.1 ASTM Standards:²

D16 Terminology for Paint, Related Coatings, Materials, and Applications

E2456 Terminology Relating to Nanotechnology

E3172 Guide for Reporting Production Information and Data for Nano-Objects

E3144 Guide for Reporting the Physical and Chemical Characteristics of Nano-Objects

2.2 ISO Standards:³

ISO 26824:2013(en) Particle Characterization of Particulate Systems – Vocabulary (1883) (1985)

ISO/TS 12805:2011(en) Nanotechnologies – Materials
 Specifications – Guidance on Specifying Nano-Objects
 ISO/TS 80004-1:2015(en) Nanotechnologies – Vocabulary –

Part 1: Core Terms 2.3 Other Documents:

The Uniform Description System for Materials on the Nanoscale CODATA-VAMAS Working Group on the De-

scription of Nanomaterials, as released on 25 May 2016⁴

 $^{^{1}}$ This guide is under the jurisdiction of ASTM Committee E56 on Nanotechnology and is the direct responsibility of Subcommittee E56.01 on Informatics and Terminology.

Current edition approved Nov. 15, 2019. Published December 2019. DOI: 10.1520/E3206-19.

² For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

³ Available from International Organization for Standardization (ISO), ISO Central Secretariat, BIBC II, Chemin de Blandonnet 8, CP 401, 1214 Vernier, Geneva, Switzerland, http://www.iso.org.

⁴ Available from Committee on Data (CODATA) International Science Council, 5 rue Auguste Vacquerie, 75016 Paris, France, https://www.codata.org/nanomaterials.

3. Terminology

- 3.1 *Definitions*—For definitions of general terms used in this standard, see *ASTM Online Terminology Dictionary of Engineering Science and Technology*.⁵
 - 3.2 Data Description Definitions:
- 3.2.1 *descriptor*, *n*—numerical data or text that expresses the measurement, observation, or calculational result of some aspect of an object..
- 3.2.1.1 *Discussion*—A descriptor conveys both the semantics of the results as well as the result itself.
- 3.2.2 *information category*, *n*—a set or group of related descriptors that represent a property, characteristic, interaction, performance, or other feature of an object.
- 3.2.2.1 *Discussion*—Information categories may be hierarchical and contain subcategories (referred to as such), each containing a set of descriptors.
- 3.2.2.2 *Discussion*—Information categories and their subcategories are constructed to convey understanding of the structure, properties, features, and performance of an object.
- 3.2.2.3 *Discussion*—A descriptor can occur in more than one information category.
- 3.2.2.4 *Discussion*—It is the responsibility of the owner of data or information resources using an information category to ensure that data and information redundancy is adequately addressed.
 - 3.3 Nanomaterials Terminology:
- 3.3.1 agglomerate, n—collection of weakly or mediumstrongly bounded nano-objects where the resulting external surface area is similar to the sum of the surface areas of the individual components.
- 3.3.1.1 *Discussion*—The forces holding an agglomerate together are weak forces, for example, van der Waals forces, or simple physical entanglement.

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- 3.3.1.2 *Discussion*—Agglomerates are also termed secondary nano-objects and the original sources of nano-objects are termed primary nano-objects.
- 3.3.1.3 *Discussion*—Adapted from ISO 26824:2013(en), 1.2, with the substitution of "nano-objects" for "particles" in the definition and the *Discussions*.
- 3.3.2 aggregate, n—comprising strongly bonded or fused nano-objects where the resulting external surface area is significantly smaller than the sum of surface areas of the individual components.
- 3.3.2.1 *Discussion*—The forces holding an aggregate together are strong forces, for example, covalent or ionic bonds, or those resulting from sintering or complex physical entanglement, or otherwise combined former primary nano-objects.
- 3.3.2.2 *Discussion*—Aggregates are also termed secondary nano-objects and the original sources of nano-objects are termed primary nano-objects.
- 3.3.2.3 *Discussion*—Adapted from ISO 26824:2013(en), 1.2, with the substitution of "nano-objects" for "particles" in the definition and the *Discussions*.
- 5 ASTM Online Terminology Dictionary of Engineering Science and Technology, available from ASTM International, ASTM Stock Number: DEFONLINE.

- 3.3.3 collection of nano-objects, n—two or more nano-objects that are associated in some way..
- 3.3.3.1 *Discussion*—The nano-objects in a collection can be physically associated, such as in an aggregate or agglomerate, or a simple grouping, such as a commercial batch of nano-objects, or some combination thereof.
- 3.3.3.2 *Discussion*—A collection of nano-objects and individual nano-objects are the two major types of nanomaterials.
- 3.3.4 *engineered nanomaterial*, *n*—nanomaterial designed for specific purpose or function.

ISO/TS 80004-1:2015(en), 2.8

- 3.3.5 *equivalency, n*—the ability of a description system to establish that two objects as assessed by different disciplines or user communities are the same according to specified criteria.
- 3.3.5.1 *Discussion*—In this guide, equivalency is the ability to establish that two nano-objects are the same according to specified criteria.
- 3.3.6 *manufactured nanomaterial*, *n*—nanomaterial intentionally produced to have selected properties or composition.

ISO/TS 80004-1:2015(en), 2.9

- 3.3.7 *nanomaterial*, *n*—material with any external dimension in the nanoscale or having internal structure or surface structure in the nanoscale. **ISO/TS 80004-1:2015(en), 2.4**
- 3.3.8 *nano-object*, *n*—discrete piece of material with one, two or three external dimensions in the nanoscale.

ISO/TS 80004-1:2015(en), 2.10

3.3.8.1 *Discussion*—The second and third external dimensions are orthogonal to the first dimension and to each other.

ISO/TS 80004-1:2015(en), 2.5

- 3.3.8.2 *Discussion*—A nano-object is the smallest unit of nanomaterial that exists as a separate functional entity.
- 3.3.8.3 *Discussion*—A multilayer structure that is the smallest unit of nanomaterial with a specific functionality is defined herein to be a nano-object (see 3.3.7). 3.206–19
- 3.3.9 *nano-object feature*, *n*—a distinctive aspect of a nano-object..
- 3.3.9.1 *Discussion*—A nano-object feature can occur anywhere within or upon the nano-object.
- 3.3.9.2 *Discussion*—Within this guide, the term *nano-object feature* is sometimes referred to simply as a *feature*.
- 3.3.10 *naturally-occurring nanomaterial*, *n*—a nanomaterial made exclusively by natural processes..
- 3.3.10.1 *Discussion*—A naturally occurring nanomaterial, when altered in any way by a process planned or controlled by humans, is, by definition, an engineered or manufactured nanomaterial.
- 3.3.10.2 *Discussion*—A nanomaterial produced by a natural process not planned or controlled by humans, for example, digestion or weathering of a rock, is naturally occurring.
- 3.3.10.3 *Discussion*—There are instances when it is ambiguous or difficult to say whether a nanomaterial is naturally occurring, engineered, or manufactured.
 - 3.3.11 *uniquely, adv*—the quality of having uniqueness..
- 3.3.12 *uniqueness*, *n*—the ability of a description system to differentiate one collection of nano-objects from every other collection of nano-objects and to establish which specific

collection of nano-objects is being described within the broad range of disciplines and user communities..

- 3.4 Physical Structure Terminology:
- 3.4.1 *physical structure*, *n*—the physical arrangement of and relationship among the parts of a collection of nano-objects..

4. Summary of Guide

- 4.1 This guide enumerates information categories and their contained descriptors used to report the physical and chemical characteristics of a collection of nano-objects. In practice, only a subset of information categories or descriptors will likely be used in each report instance.
- 4.2 Different amounts of data and information are generated in different measurement scenarios. For example, a researcher can concentrate on studying how size distribution influences the properties or functionalities of a collection of nano-objects. In this instance, the size distribution may be reported with more detailed information than for other characteristics.
- 4.3 Specifying a collection of nano-objects uniquely is critical in many applications.
- 4.3.1 For commercial transactions, specification of a collection of nano-objects uniquely ensures that a purchaser receives the desired product.
- 4.3.2 For research purposes, specification of a collection of nano-objects uniquely ensures that properties and functionalities can be correlated with true features of a collection of nano-objects as well as allowing others to duplicate research results.
- 4.3.3 For regulatory purposes, specification of a collection of nano-objects uniquely ensures that regulatory actions are applied only to the intended nano-object collection(s).

Note 1—The choice of which information categories and descriptors to be compared is dependent on the application and context and is not defined in this guide.

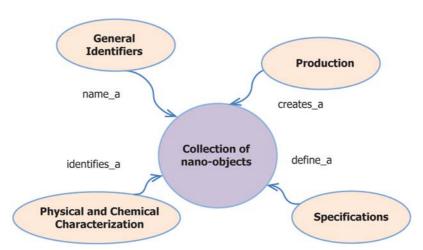
4.4 This guide can be used to determine that two collections of nano-objects are the same with respect to their physical and

chemical characteristics by comparison of the data reported using the information categories and descriptors defined herein.

4.5 When two or more collections of nano-objects are specified uniquely and determined to be equivalent, data sets of their properties and functionalities can be combined on a scientifically valid basis to create larger data collections.

5. Significance and Use

- 5.1 A nano-object is an individual, well-defined, and separable piece of a nanomaterial; in practice, nanomaterials used in research, products, testing, and other uses are almost always collections of nano-objects. Individual nano-objects and collections of nano-objects are the two major types of nanomaterials in use. The description of a collection of nano-objects is covered in this guide. The description of an individual nano-object is covered in Guide E3144. Nano-objects, individually or as a collection, are often embedded in other materials for commercial, research, and other uses. These embedded nanomaterials can be described using the information categories and descriptors included in these guides.
- 5.2 Nanomaterials are of growing importance in research and commerce, and data on their physical and chemical characteristics are critical to predict performance, to transact commercial activities, to assess their potential for harm to human and animal health and the environment in general, and to support regulations that affect their use. A collection of nano-objects is the predominant type of nanomaterial tested and used in commerce.
- 5.3 The four types of data and information used to describe a collection of nano-objects are: physical and chemical characteristics; production; specifications; and general identifiers (names and classifications), as shown in Fig. 1.
- 5.4 This guide deals solely with data and information to describe the physical and chemical characterization of a collection of individual nano-objects.



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FIG. 1 Data and Information Types Necessary to Describe a Collection of Nano-Objects

Note 2—Other guides and documents (see Section 2, Referenced Documents) deal with the data and information for production, specifications, and general identifiers (names and classifications).

Note 3—Specifications are formal or informal documents that provide guidance on specifying the composition, structure, or any other aspect of a nano-object or a collection of nano-objects.

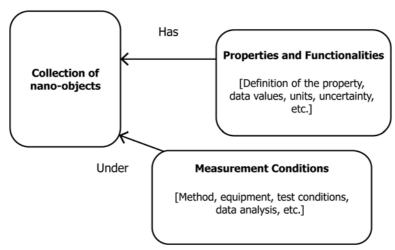
- 5.5 In a practical sense, the amount of data and information reported to describe the physical and chemical characteristics of a collection of nano-objects differs widely depending on who is reporting and the reason they are reporting. Researchers examining specific aspects of a collection of nano-objects can choose to report a limited subset of characteristics. For example, a test report on the potential toxicity of a collection of nano-objects can choose to report numerous characteristics. This guide supports both limited and complete reporting of characteristics enumerated herein.
- 5.6 The science of characterizing collections of nanoobjects is still evolving. Some information categories will require additional descriptors as new knowledge is developed. Some descriptors can become obsolete. Users should consult the latest guide for the most complete recommendations.
- 5.7 The technology for collecting, storing, analyzing, and disseminating scientific and technical data continues to evolve, and tools such as ontologies, database schemas, data repository reporting requirements, and data recoding formats are evolving similarly. This guide provides a clear, English language definition of information categories and descriptors used to describe a collection of nano-objects that can be used in these and other similar tools.
- 5.8 A collection of nano-objects has properties and functionalities that are measured under specific measurement conditions. The description of a collection of nano-objects requires data and information on its properties as well as on the conditions under which those properties were measured, as shown in Fig. 2.
- 5.9 The characteristics of a collection of nano-objects defined in this guide address the important physical and chemical properties of that collection. Because the techniques and

instruments used to measure these properties can greatly influence the property value, when available, the measurement result being used should include as much information as possible about the measurement conditions.

5.10 This guide is designed for use whenever the data and information on the physical and chemical characteristics of a collection of nano-objects are reported.

6. Collections of Nano-Objects

- 6.1 The production and use of nanomaterials can be done on a "bottoms-up" basis resulting in a single individual nanoobject, or on a "top-down" approach resulting in a collection of identical, similar, or dissimilar nano-objects. Collections of nano-objects are the subject of this guide.
- 6.2 A collection of nano-objects is created either deliberately or through natural interactions and occurs during production, shipment, testing, and use. In most cases, the reactivity of individual nano-objects means that on a practical scale, it is difficult to produce, manipulate, or use an individual nano-object in isolation of all other nano-objects.
- Note 4—There are exceptions when one considers applications such as are being explored in the manipulation of quantum dots for creating qubits for quantum computing applications, or the delivery of a drug via an individual nano-object.
- 6.3 A collection is differentiated from bulk materials with nano-objects in that a collection only contains nano-objects.
- Note 5—There remains the ambiguity of an individual nano-object that has acquired adherents such as a full corona or partial coverage. In these cases, using the information categories for an individual nano-object is preferred.
- 6.4 A collection of nano-objects can be homogeneous, composed of one type of nano-object, or heterogeneous, composed of two or more different types of nano-objects. Because of the wide diversity of possible collections, considerable thought must be given to the details of accurately describing a collection.
- 6.5 Agglomerates and aggregates of nano-objects are considered collections.



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FIG. 2 Data and Information Components Necessary to Describe a Nanomaterial and Its Properties