A Minimal Set of Characterization Parameters

Ensuring Appropriate Material Characterization in Nano-Toxicity Studies: A Workshop

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Why?

Why?

A list of chemical and physical parameters could be used for:

- Material identification
- Predictive toxicology
- Standardization/requirements for peer-reviewed publications

Examples:

Material Identification

- Composition
- Particle size / size distribution
- Shape
- Stability
- Surface area
- Surface chemistry

Predictive Toxicology

- Agglomeration state / Aggregation
- Oxidizing properties
- Particle size / size distribution
- Shape
- Surface area
- Surface chemistry
- Surface Charge

Peer-reviewed Literature

- Purity
- Composition
- Particle size / size distribution
- Shape
- Surface area
- Surface Charge

ISO-229 List

The following project is currently under development by ISO/TC 229 WG 3

ISO/TC 229 WG 3 – Health, Safety, and Environment
Project Group 5
Technical Report

Project Leader: **Richard C. Pleus, Ph.D.**

Countries Represented on Committee

Canada

Czech Republic

France

Germany

Islamic Republic of Iran

Japan

United Kingdom

United States

JWG 2 Liaison

OECD Liaison

Current Process

Draft Version November 7, 2007

Table 1 Comprehensive List of Physico-Chemical Characterization Parameters of Engineered Nanoscale Materials For Toxicologic Assessment Obtained from Selected Documents.

Characterization	Oberdorster et al. 2005[1]	Defra[2]	EPA[3]	Clancy 2007[4]	NCL[5]	DuPont[6]	Other
Agglomeration state / Aggregation	X		X	X	X	X	
Composition	X		X	X	X	X	
Solubility		X	X	X	X	X	
Concentration	X			X		The concentration of elemental chemicals or chemical compounds in the nanomaterial.	
Flammability		X	X	X			
Partition coefficient n-octanol/water		X	X	X			
Physical State			X	X		X	
Shape	X		X			X	
Size distribution	X		X		X		
Surface area	X		X	X			
Boiling Point		X	X				
Crystal structure	X		X				

Working Draft 1 *Do note cite or quote*
Draft Date: October 26, 2007 ISO/TC 229 N 254b

Current Status:
Proposed List of Physico-Chemical Characteristics of Engineered Nano-Objects for Toxicological Assessment
May 27, 2008 version

- Agglomeration state / Aggregation
- Composition (e.g., chemical composition and structure)
- Particle size / size distribution
- Purity
- Shape
- Solubility
- Stability
- Surface area
- Surface chemistry
- Surface Charge

Table 2. Focused List of Physico-Chemical Parameters of Engineered Nano-Objects for Toxicological Assessment

Characterization	Category 1 - Yes! Keep on Table	Category 2 - Maybe we should keep on Table	Category 3 - Move to Table 3	Category 4 - Remove from all lists	Category 5 - Other (not sure what to do)	Canada Renzo Comments
Agglomeration state / Aggregation	XXXXX	X				
Composition	XXXXXX					
Solubility	XXXXXX					Important to understand what is meant by solubility - do you mean, is the nanoparticle dissolving in solution? (which would be a fate consideration) or do you mean is the nanoparticle remaining suspended in solution? (which would be a compartmentization consideration).
Surface area	XXXXX	X				
Shape	XXXXXX					
Surface chemistry	XXXXX					
Zeta Potential	XXXXX	X				
Concentration	XXXXX					
Particle size / distribution	XXXXXX					
Partition coefficient n-octanol/water	XX	XX	X		X	For chemicals there is a known
Porosity	XXXX		XX			

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Next Steps

- Definitions being developed
- Measures identified
- Methods identified

- ISO/TAG needs experts to support this work and the work of the three other working groups of the TAG

The OECD juggernaut: Vertical integration on dozens of nanomaterials

- Intention is that the OECD characterization list would be reported consistently for all tests done for
  - environmental fate and transport,
  - ecotoxicity, and
  - mammalian toxicity
- For each of the “Sponsored nanomaterials” being tested.
  - Up to 14 categories of materials,
  - 2 or 3 nanomaterials in each sponsorship program
- Around 10 countries participating in testing.
- Standard setting through shear inertia….

Table of the Sponsorship Arrangements

	Lead sponsor(s)	Co-sponsor(s)	Contributor
Fullerenes(C60)	Japan United States		Denmark China
SWCNTs	Japan United States		Canada France Germany EC China BIAC
MWCNTs	Japan United States	Korea BIAC	Canada France Germany EC China BIAC
Silver nanoparticles	Korea United States	Australia* Canada Germany Nordic Council of Ministers	Australia France EC China
Iron nanoparticles	China	BIAC	Canada United States Nordic Council of Ministers
Carbon black			Denmark Germany United States
Titanium dioxide	Germany France	Canada Korea Spain United States BIAC	Denmark China
Aluminium oxide			Germany United States
Cerium oxide	United States United Kingdom/BIAC(NIA)	Netherlands	Australia Germany EC
Zinc oxide	United Kingdom/BIAC(NIA)	Australia* United States BIAC(CEFIC)	Australia Canada
Silicon dioxide	France* EC	Korea BIAC(CEFIC)	Denmark France
Polystyrene			Korea
Dendrimers		Spain	United States
Nanoclays			Denmark United States

INTERTOX

Compare Lists

Parameters	ISO DRAFT (2008)	OECD (2008)	NIST (2008)	Warheit (2008)	D. Ray (2007)
Agglomeration state / Aggregation	X	X	X	X	X
Particle size / size distribution	X	X	X	X	X
Purity	X	X	X	X	
Surface Area	X	X	X		X
Surface Chemistry	X	X	X		X
Composition (e.g., chemical composition and structure)	X	X		X	X
Shape	X	X	X		
Solubility	X	X	X		
Stability	X	X	X		
Surface Charge	X	X			X
Surface Reactivity			X	X	
Synthesis / Preparation			X	X	
Concentration (needs to be defined)		X	X		
Zeta Potential		X	X		
Crystal Structure / Crystallinity				X	X
Surface / Interfacial Energy			X		
Catalytic Properties		X			
Crystalline Phase		X			
Dustiness		X			
Fat Solubility / Oleophilicity		X			
Grain Size		X			
Water solubility / Hydrophilicity		X			
Representative TEM Picture(s)		X			
Photocatalytic Activity		X			
Pour Density		X			
Porosity		X			
Octanol-water partition coefficient		X			
Redox Potential		X			
Radical Formation Potential		X			

Parameters	ISO DRAFT (2008)	OECD DRAFT (2007)	NIST (2008)	Warheit (2008)	D. Ray (2007)
Agglomeration state / Aggregation	X	X	X	X	X
Particle size / size distribution	X	X	X	X	X
Purity	X	X	X	X	
Surface Area	X	X	X		X
Surface Chemistry	X	X	X		X
Composition (e.g., chemical composition and structure)	X	X		X	X
Shape	X	X	X		
Solubility	X	X	X		
Stability	X	X	X		
Surface Charge	X	X			X
Surface Reactivity			X	X	
Synthesis / Preparation			X	X	
Concentration (needs to be defined)			X		
Zeta Potential		X	X		
Crystal Structure / Crystallinity				X	X
Surface / Interfacial Energy			X		
Catalytic Properties		X			
Crystalline Phase		X			
Dustiness		X			
Fat Solubility / Oleophilicity		X			
Grain Size		X			
Water solubility / Hydrophilicity		X			
Representative TEM Picture(s)		X			
Photocatalytic Activity		X			
Pour Density		X			
Porosity		X			
Octanol-water partition coefficient		X			
Redox Potential		X			
Radical Formation Potential		X			

ISO Draft

DRAFT
Focus List of Physico-Chemical Characteristics of Engineered Nano-Objects for Toxicological Assessment
May 27, 2008 version

- Agglomeration state / Aggregation
- Composition (e.g., chemical composition and structure)
- Particle size / size distribution
- Purity
- Shape
- Solubility
- Stability
- Surface area
- Surface chemistry
- Surface charge

OECD

2008 OECD Guidance Manual for Sponsors, Version 1

- Agglomeration / aggregation
- Composition
- Hydrodynamic size / particle size measurement / distribution
- Purity
- Shape
- Specific surface area
- Surface chemistry
- Surface charge

- Catalytic properties
- Concentration (needs to be defined)
- Crystalline phase
- Dustiness
- Fat Solubility / oleophilicity
- Grain Size
- Length
- Water solubility / hydrophilicity
- Zeta potential

Questions We Might Ask

- Should the parameter have the ability to **reliably identify a nano-object** / Which parameters are **unique to nano**?
- Should each parameter that is to be listed have the goal of having a number generated?
- **Not all of the parameters have methods** for measuring. Is that a reason not to list?
- Should we **prioritize** the list?

Straw man approach

- Use the overlap of ISO and OECD lists
  - Keep it short for now
  - Add to it later as needed
- Endorse it as a “Journal Editors” list
  - The “MIAME” of nano
  - How? What review/endorsement is needed?
- Make ISO and OECD lists consistent and communicative
- Learn from OECD effort and have a process to revisit the ISO list and the requirements within them

Questions?