



*NSF International Standard /
Green Chemistry Institute /
American National Standard*

NSF/GCI/ANSI 355 - 2011

Greener Chemicals and Processes Information



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Chair, Joint Committee on Chemicals and Processes Information
c/o NSF International
789 North Dixboro Road, P. O. Box 130140
Ann Arbor, Michigan 48113-0140 USA
Phone: (734) 769-8010
Telex: 753215 NSF INTL
FAX: (734) 769-0109
E-mail: info@nsf.org
Web: <http://www.nsf.org>

NSF International Standard/
Green Chemistry Institute
American National Standard
for Greener Chemicals and Processes Information —

Greener Chemicals and Processes Information
Gate-to-gate information on chemical products and their manufacturing processes

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Foreword²

This American National Standard, NSF/GCI/ANSI 355 Greener Chemicals and Processes Information Standard, has been developed as part of the ongoing efforts of a number of interested parties to standardize information related to a chemical and its manufacturing processes in the molecular transformation phase of the chemical enterprise. Stakeholders involved in developing the Standard included chemical manufacturers, fabricators and formulators, end users, state and federal agencies, academics, and environmental non-governmental organizations.

The purpose of the Information Standard is to provide the chemical enterprise with a voluntary and standardized way to define and report environmental and human health hazards associated with a chemical product and its gate-to-gate manufacturing process impacts.

As used in this ANSI Standard, the term “should” indicates an optional reporting element where “shall” indicates a required reporting element.

Manufacturers of chemicals benefit by using NSF/GCI /ANSI 355 to develop one comprehensive report to satisfy many different requests for information from customers. This report serves as a basis for a normalized framework for business to business communication about chemicals throughout the supply chain.

Users of chemicals benefit by receiving a certified NSF/GCI /ANSI 355 report that contains complete, up-to-date, verified information from their suppliers and may be used as a foundation for informed decision making.

Comments on this Standard should be sent to NSF International, Standards Department, P.O. Box 130140, Ann Arbor, Michigan 48113-0140, USA or to standards@nsf.org.

² The information contained in this Foreword is not part of this American National Standard (ANS) and has not been processed in accordance with ANSI's requirements for an ANS. Therefore, this Foreword may contain material that has not been subjected to public review or a consensus process. In addition, it does not contain requirements necessary for conformance to the Standard.

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NSF International and Green Chemistry Institute
Standard for

Greener Chemicals and Processes Information

Gate-to-gate information on chemical products and their manufacturing processes

1 General

1.1 Purpose

The purpose of the Greener Chemicals and Processes Information Standard is to provide the chemical enterprise with a voluntary and standardized way to define and report the primary categories of information, their respective data elements, and data quality objectives pertaining to the relative greenness of a chemical product and its manufacturing process within one stage (i.e., gate-to-gate, as defined in 4) of its life cycle. This information shall be provided by suppliers to communicate clearly, with transparency and consistency, to help customers evaluate the relative greenness of a chemical product and process. The intent is for this information to be informative to life cycle assessments, but is not a life cycle assessment itself.

The Standard further stipulates reporting a minimum set of social responsibility criteria that are applied to the product and process claiming conformance.

For the purposes of this Standard, greener refers to the relative measure of ecosystem and human health impacts of a chemical and its process when compared to the same or similar chemical and its process.

1.2 Scope

This Standard applies to products and processes at facilities in any global location(s). Corporate-level aspects such as social responsibility apply irrespective of the location of the corporate headquarters, business incorporation, or facilities associated with the conforming product and process. Facility-level aspects are limited to only those facilities where the conforming product and process is located.

Each data element shall be addressed for both the conforming product and the process used to manufacture the product as specified by conformance pathways (optional or required) described in each section.

The scope of the Standard is limited to gate-to-gate (as defined in 4) or the molecular transformation phase of the chemical product and its processes and is depicted in 2.2.3 Establishing Process Boundaries.

1.3 Guiding premises

This Standard was developed based on the following important premises:

- 1) Reporting in conformance with this Standard is voluntary.
- 2) Data and information reported in this Standard are intended to be relevant, accurate, verifiable, and obtained, where practical, using standard methods so that users can compare reports reliably.
- 3) To the extent practical, this Standard is designed to draw from information collected and reported for other purposes, thereby minimizing the additional burden for the user.
- 4) The use of a standard set of parameters can enhance communications between suppliers and customers. This enables improved decisions about chemical product choices and can lead to and build momentum for innovation in product design, development, manufacture, use, reclamation, and disposal.
- 5) Chemical products and processes should be designed considering improved material and energy efficiency (inputs and outputs) as well as inherent properties. The environmental footprint of a chemical product is related to both the inherent properties of the chemical product itself and the environmental impact of the process(es) used to manufacture that chemical product.
- 6) Greener chemical products should be designed to preserve efficacy of function, meet customer specifications and requirements, and provide value and benefits to society, while reducing negative health and environmental impacts. Long-term, sustained acceptance and use of greener chemical product and process innovations in the marketplace depends upon meeting customer performance specifications.
- 7) End of life disposition should be considered during the design of the product. The design of chemical products should consider intended use and expected product life time, targeted durability, and reuse, recycle or beneficial disposition with the goal of getting the full functional potential during every product life stage.
- 8) Consideration of life cycle attributes throughout the value chain fosters an evaluation of long term impacts and can further stimulate the search for innovative chemical products and processes.
- 9) Although the Standard focuses on the gate-to-gate reporting of the user, it is intended to encourage continual improvement throughout the supply chain and to avoid shifting the health and environmental burden either between environmental media or up and down the value chain.
- 10) Although the Standard focuses on the inherent properties of a chemical product, it is recognized that the impact of these inherent properties should be evaluated in context of the exposure potential of each application and use of that chemical product.
- 11) Greener chemicals and processes shall not be developed at the detriment of employees or the public at large.

1.4 Relationship with laws and regulations

This Standard assumes compliance with all applicable laws and regulations. Some elements of the Standard address activities that are subject to regulation and are included here because they are key considerations for identifying greener products and processes. The Standard does not change the regulatory requirements nor does it prescribe how compliance is to be achieved. Documentation of

compliance with certain key regulations may be included in some sections of the Standard; however this does not change the underlying regulatory requirements.

1.5 International trade aspects

The procedures and requirements included within this Standard have been prepared, adopted, or applied with a view to avoid obstacles to international trade.

2 Conformance Requirements

2.1 Purpose

One objective of this Standard is to establish a set of verifiable and accurate data on chemical products and their manufacturing processes. This information is intended to be reported in a gate-to-gate, business-to-business communication to improve life cycle thinking and result in informed decisions on selecting greener chemical products in the business-to-business marketplace.

In responding to the business-to-business conversations with its customer, a manufacturer preparing the report under this Standard has the option to select self-certification, second-party certification, or third-party certification.

2.2 Intended users of this Standard

The primary intended user claiming conformance to this Standard is the chemical manufacturer who transforms discrete chemical substances into other chemical substances. Within the supply chain, this manufacturer often resides between those industries extracting materials and fabricators or formulators (see Annex A, section A.2, Chemical Enterprise). When claiming conformance to this Standard, it is critical to specify the boundaries of the process and the product for which information is reported (see 2.2.1 – 2.2.3). Others who choose to conform to this Standard shall clearly describe the product and processes for which they are reporting, explaining those data elements that may not be applicable so customers can appropriately evaluate relative greenness.

2.2.1 Gate-to-gate reporting

The report developed in conformance with this Standard is based upon gate-to-gate information (as defined in 4) on a chemical product and its related transformation and processing (see Annex A, section A.2, Chemical Enterprise); except for those parameters that are clearly identified for reporting on a facility basis as specified in this Standard.

A manufacturer shall report information associated with the transformation immediately preceding transfer of the product from the manufacturer's control (their transformation).

If the product results from a multistep process, a manufacturer should report information associated with contiguous processes under its control preceding or following the final transformation.

A manufacturer should attempt to obtain information on upstream processes not in its control so as to present a complete manufacturing picture.

Information reported shall be accompanied by a general description of all steps within the molecular transformation processes covered in the gate-to-gate unit process defined by the manufacturer.

2.2.2 Product identification

The manufacturer of the product seeking conformance shall specify information essential to the purchaser or user of the product as sold. At a minimum this essential information shall include:

- Identify trade name of chemical product
- Report Chemical Abstract Numbers and percentage range of the chemical product (standard composition as sold) including total impurities
- Identify by Chemical Abstract Numbers of intentionally added constituents down to 1000 ppm:
 - If hazard tests were performed on the product as sold, the identity of intentional constituents does not need to be declared.
 - If hazard test data is not for the product as sold, the identity of intentionally added constituents in the commercial product [or product as sold] shall also be reported.

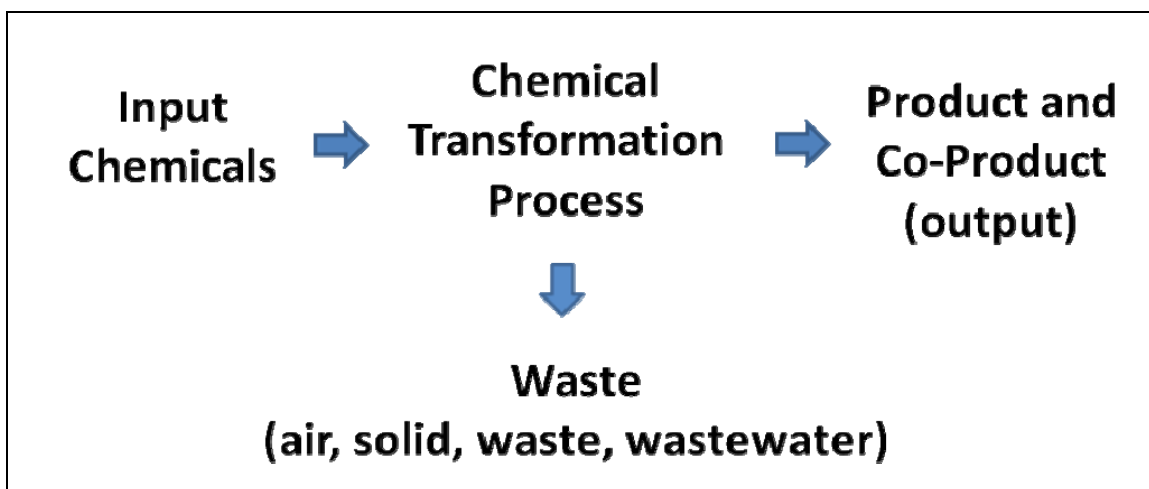
The manufacturer should consider full disclosure of all constituents when possible.

2.2.3 Establishing process boundaries

The manufacturer shall define the boundary of the unit process for the chemical product described under this Standard. The boundary for the unit process shall be used consistently throughout this Standard. The unit process may include single or multiple transformation steps. When setting the unit process boundaries, manufacturers can use guidance from life cycle standards or equivalent standards as appropriate.

Manufacturers shall provide a generalized diagram of the gate-to-gate unit process defined by the manufacturer. This generalized diagram should be sufficient for the transparent communication to the customer so that it can determine whether information and data in the reports for competing chemical products can be judged directly and comparably. A generalized diagram may be of a block-type diagram shown as Figure 1 and presented in a way that does not reveal proprietary or confidential process information. Nothing in this Standard requires the reporting of material or mass balance values and these shall not be inserted into the generalized graphic.

Figure 1 Generalized Graphic for Boundary Description



2.3 Preparing a report for conformance

2.3.1 Responsibilities of the manufacturer

The manufacturer claiming conformance to this Standard shall be responsible for the provision of data and information as specified in each section and compiled into a final report (see Annex A). The manufacturer shall (to the best of its ability) fully report data or information for each metric on a consistent unit (i.e., mass, volume-basis) and time frequency (i.e., annual) basis. These shall be identified in the final report.

It is the responsibility of the manufacturer to establish proper nondisclosure agreements and to mark their final reports appropriately to communicate to the recipients how this information can or cannot be shared.

In preparing the final report, the manufacturer shall fully document all assumptions, calculations, estimations, and/or sources of data and information provided in the final report prepared under this Standard. This documentation shall be held by the manufacturer and if appropriate, shared with the second- or third-party certifier, as requested to verify conformance with this Standard. This Standard does not mandate that the manufacturer disclose the supporting data and information in the final report to the user or customer.

2.3.2 Manufacturer guidance on communication to users/customers

The manufacturer should prepare its report for the next organization in the value or supply chain. Process data and information should be cumulatively reported to the subsequent gate-to-gate. In this way, using an additive informational module approach, a more robust set of information may be available for a future total life cycle inventory analysis.

This is a business-to-business communication covering the chemical product under commercial consideration. This Standard is based upon the premise that the customer uses many factors to make a comparative decision on which chemical product is greener given the report provided by prospective suppliers. The Standard allows each user or customer to weigh the importance of the various parameters according to its own needs.

3 References

The following documents contain provisions that, through reference, constitute provisions of this NSF/GCI/ANSI Standard. At the time this Standard was balloted, the editions listed below were valid. All documents are subject to revision, and parties are encouraged to investigate the possibility of applying the recent editions of the documents indicated below.

3.1 Normative references

Threshold Limit Values (TLVs®).³

American Chemistry Council (ACC), *Guide to the Business of Chemistry* – 2009.⁴

ANSI/API Recommended Practice 754, April 2010, *Process Safety Performance Indicators for the Refining and Petrochemical Industries*.⁵

³ American Conference of Governmental Industrial Hygienists (ACGIH®), 1330 Kemper Meadow Drive, Cincinnati, Ohio 45240, <www.acgih.org>.

⁴ American Chemistry Council (ACC), 700 Second Street NE., Washington DC 20002, <www.americanchemistry.com>.

⁵ American Petroleum Institute (API), 1220 L Street, NW, Washington, DC 20005-4070, <www.api.org>.

ASTM International (ASTM) D6866-06a, *Standard Test Methods for Determining the Biobased Content of Solid, Liquid, and Gaseous Samples Using Radiocarbon Analysis*.⁶

ASTM International E679-04, *Standard Practice for Determination of Odor and Taste Thresholds by a Forced-Choice Ascending Concentration Series Method of Limits*.⁶

Center for Chemical Process Safety of the American Institute of Chemical Engineers, *Process Safety Leading and Lagging Metrics – You Don't Improve What You Don't Measure*, 2008.⁷

Computer Assisted Evaluation of Industrial Chemical Substances According to Regulations (CAESAR).⁸

Center for Chemical Process Safety (CCPS), *Guidelines for Process Safety Metrics*, 2010.⁹

Consumer Specialty Products Association (CSPA).¹⁰

Energy Information Administration.¹¹

EN13725:2003, *Air Quality – Determination of Odour Concentration by Dynamic Olfactometry*.¹²

Federal Trade Commission (FTC), *Greenhouse Gas Reporting Rule*, 40 CFR Part 98, 2009.¹³

Federal Trade Commission (FTC), *Guides for the Use of Environmental Marketing Claims*, 16 CFR Part 260, 2010.¹⁴

Global Reporting Initiative (GRI), *Reporting Framework*.¹⁵

Global Water Tool.¹⁶

Greenhouse Gas Protocol (GHG Protocol) Initiative, *Product Life Cycle Accounting and Reporting Standard*, November 2009.¹⁷

⁶ ASTM International, 100 Barr Harbor Drive, West Conshohocken, PA 19428-2859 <www.astm.org>.

⁷ Center for Chemical Process Safety (CCPS) of the American Institute of Chemical Engineers (AIChE), 3 Park Avenue, New York, NY 10016-5991, <www.aiche.org>.

⁸ Istituto di Ricerche Farmacologiche Mario Negri, Via Giuseppe La Masa, 19, 20156 Milano, Italy, <www.caesar-project.eu>.

⁹ John Wiley & Sons, Inc., 111 River Street, Hoboken, NJ 07030-5774, <www.wiley.com>.

¹⁰ Consumer Specialty Products Association (CSPA), 1667 K Street, NW, Suite 300, Washington DC, 20006, <www.cspa.org>.

¹¹ U.S. Energy Information Administration, 1000 Independence Ave., SW, Washington, DC 20585 <www.eia.doe.gov>.

¹² European Committee for Standardization, CENELEC Management Centre, Avenue Marnix 17, B-1000 Brussels, <www.cen.eu>.

¹³ U.S. Environmental Protection Agency (USEPA), Ariel Rios Building, 1200 Pennsylvania Avenue, N.W., Washington, DC 20460, <www.epa.gov>.

¹⁴ Federal Trade Commission (FTC), 600 Pennsylvania Avenue, NW, Washington, DC 20580, <www.ftc.gov>.

¹⁵ Global Reporting Initiative (GRI), PO Box 10039 1001 EA, Amsterdam, The Netherlands, <www.globalreporting.org>.

¹⁶ World Business Council for Sustainable Development (WBCSD).4, chemin de Conches, 1231 Conches-Geneva, Switzerland, <www.wbcsd.org>.

¹⁷ The Greenhouse Gas Protocol Initiative, World Resources Institute (WRI), 10 G Street NE Suite 800, Washington, DC 20002, <www.wri.org>.

Groundwater Glossary.¹⁸

Guide to the Business of Chemistry – 2009.¹⁹

High Global Warming Potential (GWP) Gases.¹³

Immediately Dangerous to Life or Health Concentrations (IDLH) PB-94-195047.²⁰

Institute of Environmental Sciences – CML, CMLCA 5.1, *CMLCA - Chain Management by Life Cycle Assessment*, June 2010.²¹

Intergovernmental Panel on Climate Change (IPCC), 4th Assessment.²²

International Agency for Research on Cancer (IARC), World Health Organization.²³

International Reference Life Cycle Data System (ILCD) Handbook.²⁴

International Union of Pure and Applied Chemistry (IUPAC).²⁵

ISO 14021, 1999, *Environmental labels and declarations – Self-declared environmental claims (Type II environmental labeling)*.²⁶

ISO 14025, 2006, *Environmental labels and declarations – Type III environmental declarations – Principles and procedures*.²⁶

ISO 14040, 2006, *Environmental management – Life cycle assessment – Principles and framework*.²⁶

ISO 14041, 1998, *Environmental management – Life cycle assessment – Goal and scope definition and inventory analysis*.²⁶

ISO 14043, 2000, *Environmental management – Life cycle assessment – Life cycle interpretation*.²⁶

ISO 14044: 2006, *Environmental management – Life cycle assessment – Requirements and guidelines*.²⁶

¹⁸ Groundwater Foundation, P.O. Box 22558, Lincoln, NE 68542-2558, <www.groundwater.org/>.

¹⁹ American Chemistry Council (ACC), 700 Second Street, NE, Washington DC 20002, <www.americanchemistry.com/>.

²⁰ National Institute for Occupational and Safety Health (NIOSH), Centers for Disease Control and Prevention, *Chemical Listing and Documentation of Revised IDLH Values (1995)*, 1600 Clifton Rd. Atlanta, GA 30333, <www.cdc.gov/niosh/>.

²¹ Institute of Environmental Sciences – CML, Leiden University, P.O. Box 9518, 2300 RA Leiden, The Netherlands, <www.cmlca.eu/>.

²² Intergovernmental Panel on Climate Change (IPCC), 4th Assessment, C/O World Meteorological Organization, 7bis Avenue de la Paix, C.P. 2300, CH- 1211 Geneva 2, Switzerland, <www.ipcc.ch/>.

²³ International Agency for Research on Cancer (IARC), World Health Organization, 150 Cours Albert Thomas, 69372 Lyon CEDEX 08, France, <www.iarc.fr/>.

²⁴ European Commission – Joint Research Centre, Institute for the Environment and Sustainability, Via E. Fermi 2749 I-21027 Ispra (VA), Italy, <ict.jrc.ec.europa.eu/>.

²⁵ International Union of Pure and Applied Chemistry (IUPAC), 104 T.W. Alexander Drive, Building 19, Research Triangle Park, NC 27709, <www.iupac.org>.

²⁶ International Organization for Standardization (ISO), 1 ch. De la Voie-Creuse, Case Postale 56, CH-1211 Geneva 20, Switzerland, <www.iso.org>.

ISO 14064-1, 2006, *Greenhouse gases – Part 1: Specification with guidance at the organization level for quantification and reporting of greenhouse gas emissions and removals*.²⁶

ISO 14064-2, 2006, *Greenhouse gases – Part 2: Specification with guidance at the project level for quantification, monitoring and reporting of greenhouse gas emission reductions or removal enhancements*.²⁶

ISO 14064-3, 2006, *Greenhouse gases – Part 3: Specification with guidance for the validation and verification of greenhouse gas assertions*.²⁶

Minnesota Pollution Control Agency (MPCA), *Design for Environment Toolkit: A Competitive Edge for the Future*, 1998.²⁷

National Fire Protection Association (NFPA).²⁸

National Renewable Energy Laboratory (NREL).²⁹

Organisation for Economic Co-operation and Development (OECD). *Sustainable Chemistry: Promoting the Design, Manufacture, and Use of Environmentally Benign Chemicals Through Sustainable Chemistry (or "Green Chemistry")*.³⁰

Responsible Care®³¹ (not Energy Efficiency and Greenhouse Gas Emissions).

Society of Chemical Manufacturers and Affiliates (SOCMA), ChemStewards®.³²

United Nations Framework Convention on Climate Change (UNFCCC), *Kyoto Protocol to the United Nations Framework Convention on Climate Change*.³³

United Nations, *Globally Harmonized System for Classification and Labelling of Chemicals (GHS)*, Third Revised Edition, 2009.³⁴

US Environmental Protection Agency, *IRIS Glossary, Integrated Risk Information System (IRIS)*.³⁵

US Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention.³⁶

²⁷ Minnesota Pollution Control Agency (MPCA), 520 Lafayette Road, St. Paul, MN 55155-4194, <www.pca.state.mn.us/>.

²⁸ National Fire Protection Association (NFPA), 1 Batterymarch Park, Quincy, MA 02269-7471, <www.nfpa.org>.

²⁹ National Renewable Energy Laboratory (NREL), 1617 Cole Blvd., Golden, CO 80401-3305, <www.nrel.gov>.

³⁰ Organisation for Economic Co-operation and Development (OECD), 2, rue André Pascal, 75775 Paris Cedex 16, France, <www.oecd.org>.

³¹ International Responsible Care Initiative, ICCA c/o Cefic, Avenue E. Van Vieuwenhuyse 4, box 1, B-1160 Brussels, Belgium, <www.responsiblecare.org>.

³² Society of Chemical Manufacturers and Affiliates (SOCMA), ChemStewards®, 1850 M Street NW, Suite 700, Washington, DC 20036, <www.socma.com>.

³³ United Nations Framework Convention on Climate Change (UNFCCC), P.O. Box 260124 D-53153, Bonn, Germany, <<http://unfccc.int>>.

³⁴ United Nations, 1st Ave & E 44th St., New York, NY 10017, <www.unece.org>.

³⁵ US Environmental Protection Agency, *IRIS Glossary, Integrated Risk Information System (IRIS)*, 1301 Constitution Avenue NW, Washington, DC 20005, <<http://epa.gov/NCEA/iris>>.

³⁶ US Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, 1301 Constitution Avenue NW, Washington, DC 20005, <www.epa.gov/ocsp>.

US Environmental Protection Agency, *A Review of the Reference Dose and Reference Concentration Processes*.³⁷

3.2 Informational references

The references listed below informed the development of this Standard beyond the normative references and are for reference only.

Design through the Twelve Principles of Green Engineering by Anastas, P.T., and Zimmerman, J.B., *Env. Sci. and Tech.*, 37, 5, 95- 101, 2003.

Green Chemistry: Theory and Practice, by Paul T. Anastas and John C. Warner. Oxford, UK: Oxford University Press, 1998.

ISO/CD 14067-1 (under development), *Carbon footprint of products -- Part 1: Quantification*.²⁶

ISO/CD 14067-2 (under development), *Carbon footprint of products -- Part 2: Communication*.²⁶

ISO 50001 (under development), *Energy Management Systems*.²⁶

ISO/DIS 26000 Guidance on Social Responsibility.²⁶

Responsible Care®³¹, Energy Efficiency and Greenhouse Gas Emissions.

US Department of Transportation, Federal Motor Carrier Safety Administration.³⁸

US Environmental Protection Agency, *Principles of Green Engineering*.³⁹

4 Definitions

Definitions for specific chemical characteristics are located in 5, Chemical Characteristics.

4.1 auxiliary chemicals: Chemicals used during the process to create a chemical product, such as catalysts, solvents, inhibitors, initiators, reaction terminators, and solution buffers that are not transformed to make products and co-products. Chemicals used to treat and recover chemical inputs would also count as auxiliary chemicals. Auxiliary chemicals may be components of a mixture containing the chemical product or co-product. If they are neither recycled nor reused in the process, auxiliary chemicals may become waste. Auxiliary chemicals do not include general facility maintenance and worker support materials, cleaners, degreasers, lubricants, fuels, chemicals used for treating wastes and treating water at the facility, or water used for cooling. Chemicals used to convert wastes into co-products are considered auxiliary chemicals. In the Process Mass Efficiency (PME) formula, auxiliary chemicals = A (see 6.2.1 and Annex C).

4.2 bio-based carbon content: The amount of carbon in an organic chemical composed in whole or part from biological sources, forestry or agricultural materials which includes plant, animal, or marine sources.

³⁷ US Environmental Protection Agency, *A Review of the Reference Dose and Reference Concentration Processes*, Risk Assessment Forum, Washington, DC, EPA/630/P-02/002F, <<http://cfpub.epa.gov/ncea/>>.

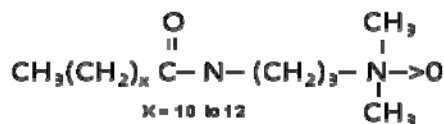
³⁸ US Department of Transportation, Federal Motor Carrier Safety Administration, 1200 New Jersey Avenue SE, Washington, DC 20590, <www.fmcsa.dot.gov>.

³⁹ US Environmental Protection Agency, *Green Engineering Principles*, 1301 Constitution Avenue NW, Washington, DC 20005, <www.epa.gov/oppt/greenengineering/index.html>.

This is measured as fraction weight (mass) or percent weight (mass) of the total carbon. It can be determined experimentally by ASTM D6866 or calculated from the carbon(s) in a chemical structure.

$$\% \text{ bio-based carbon content} = \text{bio-based carbon (mass)} / \text{total carbon (mass)} * 100$$

For example, the calculation for a chemical structure is:



	Bio-based Source			Non-Bio-based source		Bio-based carbon content
	CH ₃	(CH ₂) ₁₁	C=O	-NH(CH ₂) ₃ N(CH ₃) ₂	O	Total number of bio-based organic carbons divided by total organic carbons
Number of organic carbons	1	11	1	5	0	(13 ÷ (13 + 5))*100 = 72%

4.3 by-product: Any output(s) from a manufacturing process, chemical reaction, or biochemical pathway that is not the chemical product. By-products are either 1) used and have marketable economic value or 2) considered waste. For the purposes of this Standard, by-products that are used or sold other than for energy recovery are defined as co-products. See co-product and waste definitions.

4.4 carbon dioxide equivalents: Carbon dioxide equivalents (CO₂e) provide a universal standard of comparing the impacts of releasing (or avoiding the release of) different greenhouse gases. Conversion factors for fuel type to CO₂ equivalent are provided by governmental sources, such as those in Energy Information Administration,¹¹ or equivalent.

4.5 chemical manufacturer: A chemical manufacturer creates products by transforming organic and/or inorganic raw materials with chemical processes to different chemicals.

4.6 chemical product: The primary chemical substance that is intentionally formed for commercial use and is the result of a chemical transformation reaction. Chemical products are described by one or more chemical identification numbers (e.g., Chemical Abstract Service Registry Numbers or comparable registry numbers). In the PME formula, chemical product = P (see 6.2.1 and Annex C). For purposes of this Standard, an intentional mixture formed by blending or physical combinations (e.g., a formulation or preparation) is not considered a chemical product.

4.7 chemical process: A term broadly used to include the operations, equipment, and technology needed for chemical production, including reactors, distillation tanks, piping, boilers, cooling towers, refrigeration systems, etc. (adapted from CCPS definition of chemical process) (see Annex C). Any resources and emissions from operations used to treat waste are outside the scope/boundary of the chemical process. This would include operations such as incineration, wastewater treatment, vent treatment, etc.

4.8 company: The operating company and/or any of its divisions, and/or any of its consolidated affiliates.

4.9 co-product: A by-product of a chemical reaction with market or commercial value and that is used as a raw material and/or as a feedstock for other process reactions. The co-product may be sold as is or contains other mixtures with economic value recovered from the chemical process. For the

purposes of this Standard, a chemical recovered for use as fuel (for energy recovery) is *not* a co-product; it is a waste. Co-product is distinct from the chemical product. In the PME formula, co-product = Q (see 6.2.1 and Annex C).

4.10 energy: Any material substance or form of energy, such as electricity or steam that can be consumed to supply heat or power. Included are petroleum, coal, natural gas, and any fossil fuel derivative, renewable energy, nuclear, and any other consumable material. For purposes of this Standard, the definition of energy does not include energy used for transportation.

4.11 facility: All buildings, equipment, structures, and other stationary items that are co-located on a single property or on contiguous or adjacent properties and that are owned or operated by the same person or organization (or by any person who controls, is controlled by, or under common control with such person). Also called a site. A facility may contain more than one production plant.

4.12 freshwater: Water that contains less than 0.5 parts per thousand (500 ppm) of dissolved salts¹⁸.

4.13 freshwater use: The quantity of freshwater used in the chemical process, including water that is evaporated for cooling purposes, evaporated from water storage facilities, lost via transmission, and used directly in the product.

4.14 gate-to-gate: The segment of a product's life cycle under the control of the reporting manufacturer. Gate-to-gate spans from the first use of input materials in the transformation process, through the transformation of those materials into the chemical product that is the subject of the conformance report for a customer. The use and ultimate disposal of the chemical product outside of the reporting manufacturer's control is not included in the definition of gate-to-gate and, thus, is excluded from reporting under this Standard.

4.15 Global Warming Potential (GWP): The ratio of heat trapped by one unit mass of greenhouse gas to heat trapped by one unit mass of CO₂ over a specified time period. The concept of a global warming potential (GWP) was developed to compare the ability of each greenhouse gas to trap heat in the atmosphere relative to another gas. For purposes of reporting under this Standard, users should use Intergovernmental Panel on Climate Change (IPCC) 100 year GWP (listed in IPCC's Second Assessment Report to be consistent with the international standards under the United Nations Framework Convention on Climate Change [UNFCCC] [IPCC²², 1996]) or, if a GWP is not available for a particular greenhouse gas, the report shall specify the GWP value used for calculations⁴⁰.

NOTE - The Intergovernmental Panel on Climate Change (IPCC) has published reference values for GWPs of several greenhouse gases. Although the most current estimates for GWPs are listed in the IPCC's Third Assessment Report, EPA analyses use the 100-year GWPs listed in the IPCC's Second Assessment Report to be consistent with the international standards under the United Nations Framework Convention on Climate Change (UNFCCC) (IPCC, 1996). (See the table titled Global Warming Potentials and Atmospheric Lifetimes⁴¹ for a listing of GWPs and atmospheric lifetimes of methane and the other major species of greenhouse gases for comparison.)

4.16 graywater: Water that is collected on site from rain-water dikes, process wash-outs, and general wet clean-up that can be treated and reused.

4.17 greenhouse gas emissions: Emissions of carbon dioxide (CO₂); methane (CH₄); nitrous oxide (N₂O); sulfur hexafluoride (SF₆), and other high-GWP greenhouse gases. The definition of greenhouse

⁴⁰ High Global Warming Potential (GWP) Gases, US Environmental Protection Agency, Office of Atmospheric Programs, Climate Change Division, 1301 Constitution Avenue NW, Washington, DC 20005 <www.epa.gov/climatechange/index.html>.

⁴¹ Global Warming Potentials and Atmospheric Lifetimes, US Environmental Protection Agency, Office of Atmospheric Programs, Climate Change Division, 1301 Constitution Avenue NW, Washington, DC 20005, <www.epa.gov/nonco2/econ-inv/table.html>.

gas (GHG) emissions for purposes of this Standard is consistent with the latest IPCC²² assessment (Table 2.14). Emissions of greenhouse gases are reported in terms of carbon dioxide equivalents (CO₂e).

4.18 input chemicals: Chemicals introduced into the chemical process from outside the process. They may be purchased from a third party or transferred from another facility or supplied from products or co-products of other processes at the same facility. The mass of input chemicals is defined as the mass of reactants and auxiliary chemicals minus the mass of recycled or reused reactants and auxiliary chemicals (as used in PME calculation, 6.2.1 and Annex C).

4.19 intermediates: Chemical transformation products formed in the middle steps in a series of chemical reactions and intended to be further transformed into different product and co-product output¹⁹.

4.20 impact adjusted water: The volume of water that has been evaluated relative to local stressors using a tool such as the World Business Council for Sustainable Development's Global Water Tool¹⁶. This tool assesses a company's water use with validated water and sanitation availability information on a country and watershed basis.

4.21 life cycle inventory analysis: Phase of life cycle assessment involving the compilation and quantification of inputs and outputs for a given product system throughout its life cycle (ISO 14040)²⁶.

4.22 life cycle: Consecutive and interlinked stages of a product system, from raw material acquisition (extraction or harvesting) to final disposition (ISO 14025)²⁶.

4.23 organic carbon: Carbon atoms that make up an organic chemical. It may include non bio-based carbon or bio-based carbon.

4.24 organic chemical(s): Compounds containing carbon based compound(s) in which the carbon is attached to the other carbon atom(s), hydrogen, oxygen, or other elements in a chain, ring, or three dimensional structure (IUPAC²⁵).

4.25 other water: Brackish water (i.e., mixed fresh and salt water) or salt water that contains over 0.5 parts per thousand of salt minerals.

4.26 process: For the purpose of this Standard, process means a chemical process.

4.27 process mass efficiency (PME): The mass of input chemicals divided by the mass of output chemical product(s) (P) and any co-product(s) (Q) (see 6.2.1.2 – Calculation and Annex C).

4.28 process safety event or incident: An unplanned or uncontrolled release of material or energy due to loss of primary containment that results in one or more consequences defined in a process safety program.

4.29 process safety event or incident rate: The total number of incidents and events times 200,000 divided by total work hours during the time the incidents and events occurred.

4.30 product: For purpose of this Standard, product means “chemical product” (see chemical product 4.6).

4.31 reactant: A raw material input (natural, synthetic, or renewable) to a chemical process that is intended to be chemically transformed into a chemical product by breaking and forming chemical bonds. Auxiliary materials are not reactants. In the PME formula, reactant = R (see 6.2.1 and Annex C).

4.32 recovered energy: Energy that would have been disposed of as waste but instead has been collected through a managed process. For the purposes of this Standard, recovered energy should meet the qualifications in ISO 14021:1999(E) requirement 7.6, or their equivalent.

4.33 renewable energy: Energy produced from solar (thermal and electric), wind, biomass, landfill gas, ocean (tidal, wave, current, and thermal), geothermal, municipal solid waste, or hydroelectric sources. Renewable energy is a sustainable energy resource²⁹.

4.34 test substance: The identity of the chemical product for which the chemical characteristics test data have been generated. Where possible the purity, percentages of known impurities, and details of mixture with any adjuvant or diluent vehicle used in conducting the test should be given. If the chemical used in the specific test was different from the commercial product (purity, additives, different solvent carrier, etc), then those differences shall be noted.

4.35 waste: Outputs from chemical processes that are not considered products or co-products and are not recycled or reused. Wastes used as fuel are *not* co-products but are recovered energy and for purposes of this Standard are considered waste. Waste is disposed of or released to the environment; it may be treated on- or off-site. Waste can include such unrecovered chemicals as products, co-products, raw materials, intermediates, auxiliary materials, or by-products. Waste includes greenhouse gases and ash produced by burning or incineration and other by-products of treatment such as wastewater sludge.

4.36 wastewater treatment: Any of the mechanical, biological, or chemical processes used to improve the quality of wastewater to make it more compatible with or allow for reuse or discharge to the environment.

5 Chemical Characteristics

5.1 Purpose

As chemicals are used in the design, development, and manufacture of greener chemical products, knowledge of certain characteristics become important when making comparative decisions among differing chemicals or suppliers. Chemical characteristics are an important factor to consider when choosing chemicals for a particular product or process. Other factors, which are not addressed in this Standard, include matching chemicals to a product's desired performance attributes and cost.

5.2 Scope

It can be difficult to know if a greener chemical product or process has been developed without using standardized criteria against which alternatives are assessed. This Standard recognizes that certain chemical characteristics are in wide use while others are emerging. It is recognized that certain pieces of information are more important for the initial evaluation about chemical choices. This section of the Standard (and Annex G) highlights the rationale for the inclusion of chemical characteristics in each criteria tier, and highlights the chemical characteristics included. Each of these characteristics is discussed in the sections below. The Standard recognizes that these chemical characteristics and associated criteria may be modified as the scientific understanding of the potential environmental, human health, or safety impacts associated with chemicals evolves. This Standard is intended to be a dynamic and evolving document that reflects the most current scientific understanding.

5.3 Characteristic differentiation

For purposes of the Standard, a "chemical characteristic" describes an inherent hazard parameter of a chemical or substance that has been classified into one of three tiers (see Annex G Tier Criteria) that prescribe different levels of applicability in this Standard: Tier I - Chemical Characteristics (see Annex E Tier I references), Tier II - Emerging Characteristics (see 5.6), and Tier III - Potential Characteristics (see Annex G).

Users must report on Tier I - Chemical Characteristics (5.4) and Tier II - Emerging Chemical Characteristics (5.6).

5.4 Tier I chemical characteristics

The Tier I Chemical Characteristics are presented in three groupings: Human Health Effects, Ecological Impacts and Physical Safety Properties. This Standard identifies characteristics within these three groups and qualified tests or methods used to assess that effect or impact. Where results from multiple tests exist, as many as possible should be reported with references recognizing that data for each and every test option may not be available for every test or method. For purposes of this Standard, this applies to existing data.

Relevant information may be obtained by a search of the literature, government published data, chemical suppliers, by direct testing, or use of “scientifically robust category” and/or Quantitative Structure-Activity Relationships (QSAR) models. Use of category and QSAR approaches should be consistent with guidance prepared by EPA or the OECD³⁰. The use of intelligent testing protocols (also known as “tiered”, “phased”, or “tailored” testing) is well established in the evaluation of chemical substances for regulatory purposes. The references in Annex E provide an illustrative overview of the subject in the scientific literature, as well as its codification into chemical regulation. For example, an indicator test provides information needed to determine if additional tests are warranted, i.e., the findings from the Subchronic Animal Test(s) provide triggers for further testing relating to a range of endpoints including chronic toxicity or carcinogenicity, reproductive toxicity (e.g., reproductive organs targeted), immunotoxicity, organ effects, or neurotoxicity.

5.4.1 Human health effects

Detail for each duration and pathway are listed below.

5.4.1.1 Acute

5.4.1.1.1 Acute Inhalation – Immediately Dangerous to Life or Health (IDLH): An airborne concentration of any toxic, corrosive or asphyxiant substance that poses an immediate threat to life or would cause irreversible or delayed adverse health effects or would interfere with an individual's ability to escape from a dangerous atmosphere.²⁰

5.4.1.1.2 Acute Inhalation – Threshold Limit Value (TLV)/Short-term Exposure Limit (STEL)/Ceiling: American Conference of Governmental and Industrial Hygienists' Threshold Limit Value Short-Term Exposure Limit (STEL): a 15-minute time-weighted-average exposure that should not be exceeded at any time during a workday nor for exposure more than 4 times daily with a 60-minute rest period between each STEL exposure.³

5.4.1.1.3 Acute Inhalation – Inhalation, Lethal Concentration (LC₅₀): An LC₅₀ value is the concentration of a material in air that results in 50% mortality in the population of test animals, (typically mice or rats) following a single exposure (typically 1 or 4 hours). This value indicates the relative toxicity of the material, and applies to vapors, dusts, mists and gases³⁴. For the purposes of this Standard, the classification criteria for reporting shall be consistent with that of the GHS chapter 3.1 or equivalent.

5.4.1.1.4 Acute Dermal – Dermal, Lethal Dose (LD₅₀): The LD₅₀ (median lethal dose), dermal, is a dose of a substance applied one time to the skin that results in 50% mortality in a population of test animals. The LD₅₀ value is expressed in terms of weight of test substance per unit weight of the animal (mg/kg)³⁴. For the purposes of this Standard, the classification criteria for reporting shall be consistent with that of the GHS chapter 3.1 or equivalent.

5.4.1.1.5 Acute Dermal – Skin Irritation: The production of reversible inflammatory changes in the skin following the application of a test substance for up to 4 hours.³⁴ For the purposes of this Standard, the classification criteria for reporting shall be consistent with that of the GHS chapter 3.2 or equivalent.

5.4.1.1.6 Acute Dermal – Eye Irritation: The production of reversible inflammatory changes in the eye of a test animal following the application of a substance to the interior surface of the eye³⁴. For the

purposes of this Standard, the classification criteria for reporting shall be consistent with that of the GHS chapter 3.2 or equivalent.

5.4.1.1.7 Acute Oral – Oral, Lethal Dose (LD₅₀): The oral LD₅₀ represents the oral dose of a solid or liquid that results in 50% mortality in the population of test animals (e.g., rats, mice).³⁴ For the purposes of this Standard, the classification criteria for reporting shall be consistent with that of the GHS chapter 3.1 or equivalent.

5.4.1.2 Chronic

5.4.1.2.1 Subchronic – 28- or 90-day animal test: Repeated dose toxicity testing, typically using oral administration of a test substance in rodents for 28 or 90 days, used to predict the type of chronic toxic effects that might occur with longer-term exposures, primarily effects on various organ systems, and to establish a NOAEL. Depending on the potential route of anticipated human exposure to the substance, similar testing using dermal and inhalation dosing may also be assessed. Doses are selected to be sub-lethal but still cause toxic effects.³⁴ For the purposes of this Standard the repeat dose 28- or 90-day animal study should be accompanied by target organ pathology and the reporting shall be consistent with the GHS chapter 3.9 (specific target organ toxicity, repeated exposure) or equivalent.

5.4.1.2.2 Chronic – Reproductive or developmental effects: Reproductive or developmental effects are typically determined in special, repeat dose subchronic or chronic animal reproduction studies. Effects may include paternal or maternal reproductive effects, fertility rates, and developmental effects on the embryo, fetus and newborn.^{30,34} For the purposes of this Standard, information is reported if triggered by repeat dose testing (28 or 90 day), (GHS Chapter 3.7, Categories 1 or 1A) or a reproductive screening assay, or if indicated by QSAR. Methods include OECD 414, OECD 416 or equivalents.

5.4.1.2.3 Chronic – Carcinogenicity: The potential for a chemical to produce cancer is typically evaluated in multi-year, or lifetime, rodent studies (rats or mice). A few chemicals have been classified as human carcinogens based upon epidemiological studies, usually in studies with workers exposed for long durations.³⁴ For the purposes of this Standard, information is reported if the chemical is listed by IARC²³ or NTP or if triggered by repeat dose (GHS Chapter 3.6, Categories 1 or 1A) **and** positive results in *in vivo* genotoxicity tests (GHS Chapter 3.5, Categories 1A, 1B or 2).

Thus carcinogenic potential may be identified from results of epidemiological studies, from results of animal experiments combined with results from *in vivo* genotoxicity testing, and/or other appropriate means that may include (QSAR) analyses and/or extrapolation from structurally similar substances (read-across).⁸

5.4.1.2.4 Chronic Inhalation – Threshold Limit Value (TLV)/Time Weighted Average (TWA): The airborne concentration of a substance below which all workers are believed to be protected while exposed to it day after day for 8-hour periods. For gases and vapors, TLV/TWA is stated as parts per million (PPM) of surrounding air, and for fumes, mists, and dusts as milligrams per cubic meter (mg/m³) of surrounding air.^{3,42}

5.4.1.2.5 Chronic Inhalation – Reference Concentration (RfC): An estimate of a continuous inhalation exposure concentration (including sensitive subgroups) that is likely to be without risk of deleterious effects during a lifetime in humans. An RfC is reported in milligrams of pollutant per cubic meter of air (mg/m³).^{35,37} It is typically set based on a NOAEL value identified in a repeat dose toxicity study, followed by application of extrapolation factors to account for uncertainty due to differences in response between species and among individuals in the population (susceptible subgroups such as children).

⁴² Three categories of TLVs[®] are specified: time-weighted average (TWA); short-term exposure limit (STEL); and a Ceiling (C). For most substances, a TWA alone or with a STEL is relevant. For some substances (e.g., irritant gases), only the TLV–Ceiling is applicable. If any of these TLV[®] types are exceeded, a potential hazard from that substance is presumed to exist.

5.4.1.2.6 Chronic Oral – Reference Dose (RfD): This is an estimate, of a daily oral exposure that is likely to be without an appreciable risk of deleterious effects during a lifetime in a human population (including sensitive subgroups).^{35,43} It is typically set based on a NOAEL value identified in a repeat dose toxicity study, followed by application of extrapolation factors to account for uncertainty due to differences in response between species and among individuals in the population (susceptible subgroups such as children).

5.4.1.3 Other

5.4.1.3.1 Neurotoxicity: Chronic Neurotoxicity occurs when exposure to a material alters the normal activity of the nervous system. Neurotoxic effects may be observed in acute, subchronic, and/or chronic toxicity tests. Symptoms may appear immediately after exposure or be delayed. Some neurotoxic symptoms are reversible, while others are irreversible. Some effects are only evident after exposure of animals in utero or during postnatal development, periods of particular sensitivity for brain development. Such effects in subchronic studies in rodents or in prenatal developmental studies in rodents may include limb weakness or numbness; loss of memory, vision, and/or intellect; headache; cognitive and behavioral problems (OECD³⁰ 424 and 426).⁴⁴

5.4.1.3.2 Genotoxicity: *In vitro* tests that evaluate the potential for a chemical to disturb the hereditary mechanisms in cells or organisms so that subsequent cellular divisions produce cells that are altered in function, appearance, or survivability. For the purposes of this Standard, information is reported if the substance meets hazard classification for the bacterial reverse mutation assay (OECD 471) and in vitro cytogenetics ((OECD 473 or OECD 476) consistent with GHS³⁴ Chapter 3.5, Categories 1A, 1B, or 2). In vivo genotoxicity, studies would be needed before a carcinogenicity study is triggered for performance.

5.4.1.3.3 Sensitization (Inhalation/Dermal): A delayed allergic reaction (including itching, stinging, redness, and/or blistering) in normal animal or human tissue after repeated exposure. Eye redness and breathing difficulties may also occur.³⁴ For the purposes of this Standard, the classification criteria shall meet the definitions in GHS chapter 3.4, Category 1 using the appropriate test methods referenced in GHS or equivalent.

5.4.2 Ecological effects

5.4.2.1 Persistence, Air – Photodegradation: The chemical transformation of a compound into smaller compounds caused by the absorption of ultraviolet, visible, or infrared radiation (light).^{25,36}

5.4.2.2 Persistence, Water – Degradability - Rapidly degradable 28 day test: There are two types of aquatic degradability: biotic (e.g., biodegradation) or abiotic (e.g., hydrolysis). For the purposes of this Standard, GHS³⁴ 4.1.2 provides classification criteria for substances that shall be reported and GHS Annex 9 Appendix V, 3 provides a listing of appropriate test guidelines for biotic and abiotic degradation. Chemical classification in GHS 4.1.2.11.3 indicates the criteria for rapid degradation in the environment.⁴⁵

5.4.2.3 Persistence, Water – Photolysis: The splitting or decomposition of a chemical compound by means of light energy or photons, which should be determined using OCSP³⁶ (formerly OPPTS) 835.2110 or its equivalent.

⁴³ *Reference Dose (RfD): Description and Use in Health Risk Assessments*, IRIS, <www.epa.gov/iris/>.

⁴⁴ EPA/630/R-95/001F, *Guidelines for Neurotoxicity Risk Assessment*, 1998. **63**(93): p. 26926-26954, <www.epa.gov/iris/>.

⁴⁵ Rapid degradability can be defined under GHS using biodegradability tests (A-F) of OECD Test Guideline 301 [or its sequel, Guideline 310] or the companion OECD Test Guideline 306 for marine environments or a ratio of BOD (5 day)/COD.

5.4.2.4 Persistence, Soil – Biodegradability: A biodegradable product has the ability to break down, safely and relatively quickly, by biological means, into the raw materials of nature and disappear into the environment.

5.4.2.5 Bioconcentration Factor (BCF) - Water: This is the concentration of test material in or on fish or specified tissues thereof divided by the concentration of the chemical in the surrounding medium at steady state. In the context of setting exposure criteria it is generally understood that the terms “BCF” and “steady-state BCF” are synonymous. A steady-state condition occurs when the organism is exposed for a sufficient length of time that the ratio does not change substantially. OECD Test Guideline 305 provides the methodology for measuring bioconcentration factor.³⁰

5.4.2.6 Bioaccumulation Potential – Water⁴⁶: Evaluates the tendency for a substance to accumulate in the tissue of an aquatic or human food chain organism and forms one component of the toxicity/persistence/bioaccumulation and toxicity/mobility/persistence/bioaccumulation factors within the human food chain threat - waste characteristics factor category. The potential for bioaccumulation would normally be determined by using the octanol/water partition coefficient (usually reported at log K_{OW}) determined by OECD Test Guideline 107 or 117³⁰. An experimentally determined bioconcentration factor (BCF) provides a better measure and is preferred. OECD Test Guideline 305 provides methodology for measuring the bioconcentration factor.³⁰

NOTE – It is recognized that an aquatic BCF is an indicator of bioaccumulation in aquatic and terrestrial food webs. It is possible that a substance with a low aquatic BCF may bioaccumulate in air-respiring organisms.

5.4.2.7 Exposure, Air – Volatilization (Fugacity, Henry’s Law): Henry’s Law states that when a liquid and gas remain in contact, the weight of the gas that dissolves in a given quantity of liquid is proportional to the pressure of the gas above the liquid. This is the measure of the tendency of a substance to prefer one phase (liquid, solid or gas) over another. The phase with the lowest fugacity is the most favorable, and has the lowest Gibbs free energy. The fugacity model uses a chemical’s physical/chemical properties, including Henry’s Law and degradation half-life for air, to provide information on environmental partitioning and intermedia transport.

5.4.2.8 Exposure, Water – (Fugacity, K_{OW}): Fugacity is the measure of the tendency of a substance to prefer one phase (liquid, solid or gas) over another. The phase with the lowest fugacity is the most favorable, and has the lowest Gibbs free energy. The fugacity model uses a chemical’s physical/chemical properties, including water solubility and degradation half-life for water, to provide information on environmental partitioning and intermedia transport.

The octanol-water partition coefficient (log K_{OW}) is the ratio of the concentration of a chemical in octanol and in water at equilibrium and at a specified temperature, and is used in many environmental studies to help determine the fate of chemicals in the environment. Log K_{OW} is a measure of the lipophilicity of a substance and is a key parameter in assessing environmental fate, such as the sorption to soil and sediment and bioconcentration in organisms. Experimentally, Log K_{OW} should be performed using a variety of test guidelines indicated in GHS Annex 9, Appendix III, Section 2.

5.4.2.9 Exposure, Soil – (Fugacity, K_{OC}): The organic carbon partition coefficient (K_{OC}) is the ratio of the amount of chemical absorbed per unit of organic carbon in the soil to the concentration of the chemical in aqueous solution at equilibrium. Fugacity is the measure of the tendency of a substance to prefer one phase (liquid, solid or gas) over another. The phase with the lowest fugacity is the most favorable, and has the lowest Gibbs free energy. The fugacity model uses a chemical’s physical/chemical

properties, including K_{OC} and degradation half-life for soil, to provide information on environmental partitioning and intermedia transport.

⁴⁶ See Annex F, Bioaccumulation.