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# StandardGuide for Assessing the Environmental and Human Health Impacts of New Energetic Compounds[1]

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## INTRODUCTION

Sustaining training operations while maintaining force health is vital to national security. Research efforts are underway to identify energetic substances that have negligible environmental impacts and implement them in military munitions. This guide is intended to provide a standardized method to evaluate the potential environmental impacts of prospective candidate energetic substances. This guide is intended for use by technical persons with a broad knowledge of risk assessment, fate and transport processes, and toxicology to provide recommendations to the research chemist or engineer regarding the environmental consequences of use.

## 1. Scope

1.1 This guide is intended to determine the relative environmental influence of new munition constituents, consistent with the research and development (R&D) level of effort and is intended to be applied in a logical, tiered manner that parallels both the available funding and the stage of research, development, testing, and evaluation. Specifically, conservative assumptions, relationships, and models are recommended early in the research stage, and as the munition technology is matured, empirical data will be developed and used. Munition constituents may include fuels, oxidizers, explosives, binders, stabilizers, metals, dyes, and other compounds used in the formulation to produce a desired effect. Munition systems range from projectiles, grenades, rockets/missiles, training simulators, smokes and obscurants. Given the complexity of issues involved in the assessment of environmental fate and effects and the diversity of the munition systems used, this guide is broad in scope and not intended to address every factor that may be important in an environmental context. Rather, it is intended to reduce uncertainty at minimal cost by considering the most important factors related to the environmental impacts of energetic materials. This guide provides a method for collecting data useful in a relative ranking procedure to provide the munition scientist with a sound basis for prospectively determining a selection of candidates based on environmental and human health criteria.

1.2 The scope of this guide includes:

1.2.1 Energetic materials and compositions in all stages of research, development, test and evaluation.

1.2.2 Environmental assessment, including:

1.2.2.1 Human and ecological effects of the unexploded energetics and compositions on the environment.

1.2.2.2 Environmental transport mechanisms of the unexploded energetics and composition.

1.2.2.3 Degradation and bioaccumulation properties.

1.2.3 Occupational health impacts from manufacture and use of the energetic substances and compositions to include load, assembly, and packing of the related munitions.

1.3 Given the wide array of applications, the methods in this guide are not prescriptive. They are intended to provide flexible, general methods that can be used to evaluate factors important in determining environmental consequences from use of the energetic substances.

1.4 Factors that affect the health of humans as well as the environment are considered early in the development process. Since some of these data are valuable in determining health effects from generalized exposure, effects from occupational exposures are also included.

1.5 This guide does not address all processes and factors important to the fate, transport, and potential for effects in every system. It is intended to be balanced effort between scientific and practical means to evaluate the relative environmental effects of munition compounds resulting from intended use. It is the responsibility of the user to assess data quality as well as sufficiently characterize the scope and magnitude of uncertainty associated with any application of this standard.

1.6 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the*

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

## 2. Referenced Documents

2.1 *ASTM Standards:*[2]

D5660 Test Method for Assessing the Microbial Detoxification of Chemically Contaminated Water and Soil Using a Toxicity Test with a Luminescent Marine Bacterium

E729 Guide for Conducting Acute Toxicity Tests on Test Materials with Fishes, Macroinvertebrates, and Amphibians

E857 Practice for Conducting Subacute Dietary Toxicity Tests with Avian Species

E943 Terminology Relating to Biological Effects and Environmental Fate

E1023 Guide for Assessing the Hazard of a Material to Aquatic Organisms and Their Uses

E1147 Test Method for Partition Coefficient (N-Octanol/Water) Estimation by Liquid Chromatography (Withdrawn 2013)[3]

E1148 Test Method for Measurements of Aqueous Solubility (Withdrawn 2013)[3]

E1163 Test Method for Estimating Acute Oral Toxicity in Rats

E1193 Guide for Conducting *Daphnia magna* Life-Cycle Toxicity Tests

E1194 Test Method for Vapor Pressure (Withdrawn 2013)[3]

E1195 Test Method for Determining a Sorption Constant ($K_{oc}$) for an Organic Chemical in Soil and Sediments (Withdrawn 2013)[3]

E1241 Guide for Conducting Early Life-Stage Toxicity Tests with Fishes

E1279 Test Method for Biodegradation By a Shake-Flask Die-Away Method (Withdrawn 2013)[3]

E1372 Test Method for Conducting a 90-Day Oral Toxicity Study in Rats (Withdrawn 2010)[3]

E1415 Guide for Conducting Static Toxicity Tests With *Lemna gibba* G3

E1525 Guide for Designing Biological Tests with Sediments

E1624 Guide for Chemical Fate in Site-Specific Sediment/Water Microcosms (Withdrawn 2013)[3]

E1676 Guide for Conducting Laboratory Soil Toxicity or Bioaccumulation Tests with the Lumbricid Earthworm *Eisenia Fetida* and the Enchytraeid Potworm *Enchytraeus albidus*

E1689 Guide for Developing Conceptual Site Models for Contaminated Sites

E1706 Test Method for Measuring the Toxicity of Sediment-Associated Contaminants with Freshwater Invertebrates

## 3. Terminology

3.1 *Definitions of Terms Specific to This Standard:*

3.1.1 *conception, n*—refers to part of the munition development process whereby molecules are designed through software and modeling efforts though not yet synthesized.

3.1.2 *demonstration, n*—refers to testing munition compounds in specific configurations that may use other substances to maintain performance specifications.

3.1.3 *engineering and manufacturing development, n*—involves the process of refining manufacturing techniques and adjusting formulations to meet production specifications.

3.1.4 *environmental, adj*—used to describe the aggregate of a receptor's surroundings that influence exposure, used in the holistic sense that may include human exposures in a variety of conditions.

3.1.5 *energetic materials, n*—chemical compounds or compositions that contain both fuel and oxidizer and rapidly react to release energy and other products of combustion. Examples of energetic materials are substances used in high explosives, gun propellants, rocket & missile propellants, igniters, primers, initiators, and pyrotechnics (for example, illuminants, smoke, delay, decoy, flare and incendiary) and compositions. Energetic materials may be thermally, mechanically, and electrostatically initiated and do not require atmospheric oxygen to sustain the reaction.

3.1.6 *munition, n*—refers to weapon systems or platforms that have a military application. Includes the use of energetic substances in addition to stabilizers, plasticizers, and other substances to the final combined formulation referred to as energetic material.

3.1.7 *production, n*—includes activities involved in the finalized manufacturing and use of the munition compound and accompanying system.

3.1.8 *synthesis, n*—process in which minute (gram) quantities of the energetic material are made, often using laboratory desktop equipment.

3.1.9 *testing and refinement, n*—includes preliminary small-scale tests to large-scale testing and range operations that require refined synthesis techniques within the research and development phase for new energetic compounds. Energetic materials may be combined with other ingredients at this stage to tailor specific performance properties.

## 4. Summary of Guide

4.1 In the evaluation of the probability of adverse environmental effects, measures of exposure are compared with measures of toxicity to evaluate relative risk. These methods and data requirements are balanced with the level of funding used in munition compound development. This guideline, therefore, provides a tiered approach to data development necessary for various levels of risk assessment. Often it results in a relative ranking of properties, not a robust estimation of exposure. Initially, physical/chemical properties necessary for fate, transport, and exposure estimation may be derived and estimated from conceptual compounds developed from computer model simulations. Quantitative structural activity relationships (QSARs) and quantitative structural property relationships (QSPRs) may be useful in estimating toxicity and



[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] The last approved version of this historical standard is referenced on www.astm.org.

chemical properties, respectively. Following successful synthesis of compounds, key properties may be experimentally determined (for example, water solubility, vapor pressure, sorption ($K_{oc}$), octanol/water partition coefficients ($K_{ow}$), boiling point, and so forth). These properties can be used in a relative manner or quantitatively to determine potential for transport and bioaccumulation. Given the expense involved, toxicity studies are tiered, where lower cost *in vitro* methods are used early in the process and more expensive *in vivo* methods are recommended later in the development process. Acute mammalian toxicity data may be generated, along with soil, water, and sediment toxicity to invertebrates (Tier I tests). Earthworm bioaccumulation tests may also be conducted, along with an evaluation of plant uptake models. At advanced stages, sublethal mammalian testing shall be conducted along with avian and other limited vertebrate toxicity tests (Tier II tests).

## 5. Significance and Use

5.1 The purpose of this guide is to provide a logical, tiered approach in the development of environmental health criteria coincident with level and effort in the research, development, testing, and evaluation of new energetic materials. Various levels of uncertainty are associated with data collected from previous stages. Following the recommendation in the guide should reduce the relative uncertainty of the data collected at each developmental stage. At each stage, a general weight of evidence qualifier shall accompany each exposure/effect relationship. They may be simple (for example, low, medium, or high confidence) or sophisticated using a numerical value for each predictor as a multiplier to ascertain relative confidence in each step of risk characterization. The specific method used will depend on the stage of development, quantity and availability of data, variation in the measurement, and general knowledge of the dataset. Since specific formulations, conditions, and use scenarios are often not known until the later stages, exposure estimates can be determined only at advanced stages (for example, Engineering and Manufacturing Development; see 6.6). Exposure data can then be used with other toxicological data collected from previous stages in a quantitative risk assessment to determine the relative degree of hazard.

5.2 Data developed from the use of this guide are designed to be consistent with criteria required in weapons and weapons system development (for example, programmatic environment, safety and occupational health evaluations, environmental assessments/environmental impact statements, toxicity clearances, and technical data sheets).

5.3 Information shall be evaluated in a flexible manner consistent with the needs of the authorizing program. This requires proper characterization of the current problem. For example, compounds may be ranked relative to the environmental criteria of the prospective alternatives, the replacement compound, and within bounds of absolute environmental values. A weight of evidence (evaluation of uncertainty and variability) must also be considered with each criterion at each stage to allow for a proper assessment of the potential for adverse environmental or occupational effects; see 6.8.

5.4 This standard approach requires environment, safety, and occupational health (ESOH) technical experts to determine the risk and energetic materials researchers to evaluate the acceptability of the risk. Generally, the higher developmental stages require a higher managerial level of approval.

## 6. Procedure

6.1 *Problem Evaluation*—The first step requires an understanding of the current problem. Often, specific attributes of existing compounds drive the need for a replacement. For example, increased water solubility may indicate a propensity of the compound to contaminate groundwater. Environmental persistence and biomagnification may cause concerns regarding exposures to predatory animals and in human fish consumption. Increased vapor pressure may lead to significant inhalation exposures in confined spaces that would increase the probability of toxicity to workers or soldiers. A sound understanding of the factors principally attributed to the environmental problem is required to focus relative evaluation of these properties. A conceptualization of potential exposure pathways given specific chemical properties can be helpful in ascertaining likelihood for adverse effects. Guide E1689 can be helpful in that regard. Table 1 provides stages of technical development of munition compounds and corresponding suggested data requirements.



**TABLE 1 Life-Cycle Munition Development Stage Relative to the Collection of Data Important to the Evaluation of Environmental Criteria**

| Developmental Stage | Action | Data Requirement |
|---|---|---|
| Conception | Computer modeling (QSAR), computational chemistry | Chem/phys properties; toxicity estimates (mammalian and ecotoxicity) |
| Synthesis | Develop experimental chemical property data; conduct relative toxicity screen | Chem/phys properties (estimate fate, transport, bioaccumulation), in-vitro mammalian toxicity screen, in-vitro ecotoxicity screen (for example, luminescent bacteria) |
| Testing | Conduct Tier I mammalian toxicity testing | Acute/subacute rodent toxicity data; in-vitro cancer screen |
| Demonstration | Conduct Tier II mammalian toxicity testing; Tier I Ecotox screening | Subchronic rodent toxicity data; aquatic/plant/earthworm assays |
| Engineering and manufacturing development | Cancer studies[A] ; Tier II Ecotox studies, evaluate plant uptake | Rodent cancer evaluation; avian, amphibian studies; plant uptake models |
| Production | Evaluate exposure and effects | No additional data required[B] |
| Storage and use | Evaluate exposure and effects | No additional data required |
| Demilitarization | Evaluate exposure and effects | No additional data required |

[A] Only necessary if in-vitro screens are predominantly positive and potential for exposure is relatively high.
[B] In certain cases, it may be necessary to verify predictions through environmental monitoring procedures.

6.2 *Conception*—At this stage of energetic material development, molecular relationships and characteristics are examined to evaluate the properties of a new material. These include molecular and electronic structure, stability, thermal properties, performance and sensitivity requirements, and decomposition pathways. Since these substances are still conceptual, no empirical data exist.

6.2.1 The predicted molecular and electronic structural properties can be used in quantitative structure-activity relationship (QSAR) or other approaches to determine chemical/physical properties relating to toxicity, fate, and transport. These properties can be gleaned from computer-modeled estimations using quantitative structure-property relationship (QSPR)-like or quantum mechanical models. The properties that are useful in estimating the extent of fate and transport include the following:

6.2.1.1 Molecular weight;

6.2.1.2 Water solubility;

6.2.1.3 Henry's law constant;

6.2.1.4 Vapor pressure;

*(1)* Liquid-phase vapor pressure;

*(2)* Solid-phase vapor pressure;

6.2.1.5 Affinity to organic carbon; sorption (log $K_{oc}$);

6.2.1.6 Lipid solubility (octanol/water coefficient; log $K_{ow}$);

6.2.1.7 Boiling point;

6.2.1.8 Melting point; and

6.2.1.9 Ionization potential.

6.2.2 When existing materials show promise as alternatives, conduct a literature search to determine first if Chemical Abstract Service (CAS) registry numbers are available. A comprehensive database available from the National Institute of Health can be used to search for this information (http://chem.sis.nlm.nih.gov/chemidplus/). These CAS numbers may then be used to search for chemical/physical property values and toxicity information without significant risk of confusion regarding synonyms. Other databases may provide information regarding chemical/physical properties and toxicity. See the suite available at http://toxnet.nlm.nih.gov/.

6.2.3 Models are available to predict environmental parameters with an inherent degree of uncertainty. It is important that this uncertainty be captured using a qualitative or semiquantitative approach (see 6.8). Examples of such models include those found in the EPI suite[4] (http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm; (**1**)[5]) and can be helpful in obtaining values.

6.2.4 Henry's law constant is calculated using the following equation:

$$H = \frac{Vp(MW)}{S} \tag{1}$$

where:

$H$ = Henry's law constant (atm·m$^3$/mol),
$Vp$ = vapor pressure (atm) at 25°C (298 K),
$MW$ = molecular weight (g/mol), and
$S$ = solubility in water (mg substance/L).

6.2.5 Octanol/water partition coefficients (log $K_{ow}$) can be predicted through the use of QSPR models. Models that predict sorption (affinity to organic carbon; log $K_{oc}$) are generally not required since log $K_{oc}$ can be predicted from log $K_{ow}$ values using the following equation:

$$K_{oc} = 10^{[0.0784+(0.7919+(\log K_{ow}))]} \tag{2}$$

where:

$K_{oc}$ = soil organic carbon-water partition coefficient (mL water/g soil), and
$K_{ow}$ = *n*-octanol/water partition coefficient (unitless).

6.2.6 QSAR approaches can also be used to estimate toxicological impact. Toxicity QSAR models can often predict many parameters before experimental toxicology testing but are dependant upon similar compounds that have toxicity data. These models produce estimates of toxicity (for example, rat subchronic no observed adverse effect levels (NOAELs)) are used to rank new energetic materials, not to evaluate them quantitatively. These methods provide a relatively fast, low-cost method for developing the minimum amount of environmental data necessary for an initial evaluation of environmental impacts. They can be used as a basis for go/no-go decisions regarding further development and can serve to focus further research. These rankings shall be based on measures of toxicity (for example, acute values such as LD50s, chronic/subchronic rat lowest observed adverse effect levels (LOAELs), and so forth). QSARs may also be used in a qualitative sense to evaluate the need for focused developmental, reproductive (for example, endocrine-like functional groups) in vivo testing. Compounds with structure suggesting specific toxicity should be qualified for further testing at advanced stages in munition development (for example, engineering and manufacturing development).

6.2.7 Following the problem evaluation procedure, pertinent properties are compared along with those of other candidate substances and, if applicable, with the currently used munition constituent marked for replacement. Estimates of the relative level of confidence (for example, high, medium, or low) shall also be assigned to each attribute. These qualifiers may be assigned a numerical weight and used in a semiquantitative approach. These substances are then ranked, evaluated based on absolute parameters, and/or assessed relative to the replacement substance configuration according to these criteria to provide the munition scientist with a prioritized list from which to focus efforts or provide general recommendations regarding their use in an environmental or occupational context or both.

6.3 *Synthesis*—Following the conceptualization and successful assessment of a new material, it must be made. Once it is shown that small amounts of a new energetic material can be produced, small-scale screening tests shall be performed to establish performance characteristics. If the material is found to be acceptable from a performance perspective, risks from an environmental and occupational perspective can be more reliably determined through experimentally determining chemical properties in small-scale tests using actual material. If the candidate is suitable for further consideration, performance



[4] EPI Suite is a trademark of ImageWare Systems, Inc. 10883 Thornmint Road San Diego, CA 92127.

[5] The boldface numbers in parentheses refer to the list of references at the end of this standard.