United States Environmental Protection Agency
Office of Pollution Prevention and Toxics Washington, DC 20460
EPA 745-B-19-007
Revised February 2019

TOXICS RELEASE INVENTORY

Guidance for Reporting and List of Toxic Chemicals within the Water Dissociable Nitrate Compounds Category

Section 313 of the Emergency Planning and Community Right-to-Know Act of 1986 (EPCRA) requires certain facilities manufacturing, processing, or otherwise using listed toxic chemicals to report the annual quantity of such chemicals entering each environmental medium. Such facilities must also report pollution prevention and recycling data for such chemicals, pursuant to section 6607 of the Pollution Prevention Act, 42 U.S.C. 13106. EPCRA section 313 is also known as the Toxics Release Inventory (TRI).

CONTENTS

LIST OF TABLES

DISCLAIMER

This guidance document is intended to assist industry with EPCRA section 313 reporting for the water dissociable nitrate compounds category. In addition to providing an overview of aspects of the statutory and regulatory requirements of the EPCRA section 313 program, this document also provides recommendations to assist industry with EPCRA reporting. These recommendations do not supersede any statutory or regulatory requirements, are subject to change, and are not independently binding on either EPA or covered facilities. Additionally, if a conflict exists between guidance on this site and the statutory or regulatory requirements, the conflict must be resolved in favor of the statute or regulation.

Although EPA encourages industry to consider these recommendations, in reviewing this document, industry should be aware that these recommendations were developed to address common circumstances at typical facilities. The circumstances at a specific facility may significantly differ from those contemplated in the development of this document. Thus, individual facilities may find that the recommendations provided in this document are inapplicable to their processes or circumstances, and that alternative approaches or information are more accurate and/or more appropriate for meeting the statutory and regulatory requirements of EPCRA section 313. To that end, industry should use facility specific information and process knowledge, where available, to meet the requirements of EPCRA section 313. EPCRA section 313 also provides that, in the absence of such readily available data, a reporting facility may make reasonable estimates to meet those EPCRA section 313 requirements. Facilities are encouraged to contact the Agency with any additional or clarifying questions about the recommendations in this document, or if the facility believes that EPA has incorrectly characterized a particular process or recommendation.

Additional guidance documents, including industry specific and chemical specific guidance documents, are also available on TRI's GuideME website:
https://ofmpub.epa.gov/apex/guideme_ext/f?p=guideme:gd-list

SECTION 1.0 INTRODUCTION

On November 30, 1994, EPA added nearly 300 chemicals and chemical categories to the list of toxic chemicals subject to reporting under EPCRA section 313. These additions are described at 59 FR 61432, and were effective January 1, 1995 for reports due July 1, 1996. The water dissociable nitrate compounds category was included in these additions. At the time of the addition, EPA indicated that the Agency would develop, as appropriate, interpretations and guidance that the Agency determines are necessary to facilitate accurate reporting for these additions. This document constitutes such guidance for the water dissociable nitrate compounds category.

Section 1.1 Chemicals within the Water Dissociable Nitrate Compounds Category

EPA is providing a list of CAS numbers and chemical names to aid the regulated community in determining whether they need to report for the water dissociable nitrate compounds category. The list includes individual chemicals within the water dissociable nitrate compounds category. If a facility is manufacturing, processing, or otherwise using a chemical which is on this list, they must report this chemical. However, this list is not exhaustive. If a facility is manufacturing, processing, or otherwise using a water dissociable nitrate compound, they must report the chemical, even if it does not appear on the list.

Section 1.2 General TRI Reporting Instructions

For general instruction regarding compliance with EPCRA section 313 requirements and form completion, please see the most recent version of the Toxic Chemical Release Inventory Reporting Forms and Instructions, available at: https://ofmpub.epa.gov/apex/guideme_ext/f?p=guideme:rfi-home.

SECTION 2.0 GUIDANCE FOR REPORTING CHEMICALS WITHIN THE WATER DISSOCIABLE NITRATE COMPOUNDS CATEGORY

Note: for the purposes of reporting under the nitrate compounds category, water dissociable means that the nitrate ion dissociates from its counterion when in solution.

Section 2.1 Chemicals within the Water Dissociable Nitrate Compounds Category

Chemicals within the nitrate compounds category are only reportable when in aqueous solution. All water dissociable nitrate compounds are included in the nitrate compounds category, including ammonium nitrate. Specifically listed section 313 chemicals *are not* included in threshold determinations for chemical categories such as the water dissociable nitrate compounds category. Specifically listed toxic chemicals are subject to their own individual threshold determinations. As of December 1, 1994, ammonium nitrate (solution) is no longer an individually listed chemical on the EPCRA section 313 list. However, ammonium nitrate is still subject to reporting under the nitrate compounds category. In addition, the aqueous ammonia from the dissociation of ammonium nitrate when in aqueous solution is subject to reporting under the ammonia listing.

Section 2.2 Determining Threshold and Release Quantities for Nitrate Compounds

The total nitrate compound, including both the nitrate ion portion and the counterion, is included in the nitrate compounds category. When determining threshold amounts, the total weight of the nitrate compound is to be included in all calculations. However, only the nitrate ion portion is to be included when determining the amount of the chemicals within the nitrate compounds category that is released, transferred, or otherwise managed in wastes.

Example 1

In a calendar year, a facility processes 100,000 pounds of ammonium nitrate (NH_4NO_3), in *aqueous solution*, which is released to wastewater streams, then transferred to a POTW. The quantity applied towards threshold calculations for the nitrate compounds category is the total quantity of the nitrate compound or 100,000 pounds. Since this quantity exceeds the 25,000-pound processing threshold, the facility is required to report for the nitrate compounds category. Under the nitrate compounds category, only the weight of the nitrate ion portion of ammonium nitrate is included in release and transfer calculations. The molecular weight of ammonium nitrate is 80.04 and the weight of the nitrate ion portion is 62.01 or 77.47 percent of the molecular weight of ammonium nitrate. Therefore, the amount of nitrate ion reported as transferred to the POTW is 77.47 percent of 100,000 pounds, or 77,470 pounds (reported as 77,000 pounds). The aqueous ammonia from ammonium nitrate is reportable under the EPCRA section 313 listing for ammonia. For determining thresholds and calculating releases under the ammonia listing, see the separate directive, *Guidance for Reporting Aqueous Ammonia* (EPA 745-B-19-002; Revised February 2019).

Example 2

In a calendar year, a facility manufactures as by-products 20,000 pounds of sodium nitrate ($NaNO_3$) and 10,000 pounds of calcium nitrate ($Ca(NO_3)_2$), both in *aqueous solutions*, and releases these solutions to wastewater streams. The total quantity of nitrate compounds manufactured by the facility is the sum of the two chemicals, or 30,000 pounds, which exceeds the manufacturing threshold quantity of 25,000 pounds. The facility therefore is required to report for the nitrate compounds category. By weight, the nitrate ion portion is 72.96 percent of sodium nitrate and is 75.57 percent of calcium nitrate. Of the 20,000 pounds of the sodium nitrate in solution, 72.96 percent or 14,592 pounds is nitrate ion, and similarly, of the 10,000 pounds of the calcium nitrate in solution, 75.57 percent or 7,557 pounds is nitrate ion. The total nitrate ion in aqueous solution released by the facility is the sum of the nitrate ion in the two solutions, or 22,149 pounds.

Section 2.3 Reporting Nitrate Compounds Generated from the Partial or Complete Neutralization of Nitric Acid

Nitric acid is an individually listed chemical on the original EPCRA section 313 list and is reported as a separate chemical if the manufacture, process or otherwise use thresholds are exceeded. The partial or complete neutralization of nitric acid results in the formation of nitrate compounds which are reported as chemicals within the nitrate compounds category if their manufacture, process or otherwise use thresholds are exceeded.

Mineral acids such as nitric acid may be present in aqueous waste streams that are sent to on-site neutralization or are discharged to a publicly owned treatment works (POTW) or other off-site treatment facility. As stated in the current version of *Toxic Chemical Release Inventory Reporting Forms and Instructions* document, on-site acid neutralization and its efficiency must be reported in Part II, section 7A of Form R (waste treatment methods and efficiency section). For purposes of reporting on Form R, EPA considers a waste mineral acid at a pH 6.0 or higher to be 100 percent neutralized (water discharges to receiving streams or POTWs are reported as zero). The nitrate compounds produced from the complete neutralization (pH 6.0 or above) of nitric acid are reportable under the nitrate compounds category and should be included in all threshold and release calculations. Two Form R reports would be required if the manufacture, process or otherwise use thresholds are exceeded for nitric acid and for the nitrate compounds category.

If the nitric acid treatment efficiency is not equal to 100 percent (pH is less than 6.0), the amount of the acid remaining in the waste stream which is released to the environment on-site or off-site must be reported in Part II of Form R. The nitrate compounds produced from the partial neutralization of nitric acid are reportable under the nitrate compounds category and should be included in all threshold and release calculations. Two reports would again be required if the manufacture, process or otherwise use thresholds are exceeded for nitric acid and for the nitrate compounds category.

2.3.1 Estimating Nitric Acid Releases

The pH of the waste stream can be used to calculate the amount of nitric acid in the stream and the efficiency of neutralization. The pH is a measure of the acidity or alkalinity of a waste stream and can be obtained readily using a pH meter or pH sensitive paper. The pH scale itself varies from 0.0 to 14.0.

The total nitric acid concentration (ionized and unionized) in pounds/gallon can be calculated by using the pH value of the solution, the molecular weight and ionization constant of the acid, and appropriate conversion factors. The total acid concentration for nitric acid for different pH values is listed in Table 2-1. The calculation of mineral acid concentrations and the derivation of Table 2-1 are discussed in a separate directive, *Estimating Releases for Mineral Acid Discharges Using pH Measurements*, and in an addendum to this directive.

The procedure outlined in this guidance document for calculating the quantity of nitrate compounds formed from the complete or partial neutralization of nitric acid can be used if nitric acid is the only mineral acid in a solution. In addition, the calculation of nitric acid releases using only pH measurements is a rough estimate. The subsequent calculation of nitrate compound releases is therefore also only a rough estimate. The estimates can be made for a waste stream with a steady pH below 6.0 or for one whose pH temporarily drops to below pH 6.0. Facilities should use their best engineering judgement and knowledge of the solution to evaluate how reasonable the estimates are.

Table 2-1: Nitric Acid Concentration Versus pH

pH	Nitric Acid Concentration (lb/gal)
0.0	0.5200000
0.2	0.3300000
0.4	0.2100000
0.6	0.1300000
0.8	0.0830000
1.0	0.0520000
1.2	0.0330000
1.4	0.0210000
1.6	0.0130000
1.8	0.0083000
2.0	0.0052000
2.2	0.0033000
2.4	0.0021000
2.6	0.0013000
2.8	0.0008300
3.0	0.0005200
3.2	0.0003300
3.4	0.0002100
3.6	0.0001300
3.8	0.0000830
4.0	0.0000520
4.2	0.0000330
4.4	0.0000210
4.6	0.0000130
4.8	0.0000083
5.0	0.0000052
5.2	0.0000033
5.4	0.0000021
5.6	0.0000013
5.8	0.0000008
6.0	0.0000005

Example 3

In a calendar year, a facility transfers 1.0 million gallons of a solution containing nitric acid (HNO_3), at pH 4.0, to a POTW. Using Table 2-1, a pH of 4.0 corresponds to a concentration of 0.0000520 lb HNO_3/gallon of solution.

The weight of HNO_3 transferred can be estimated using the equation:

Transfer of HNO_3 = (concentration of HNO_3,) × (effluent flow rate)

Substituting the example values into the above equation yields:

Transfer of HNO_3 = 0.0000520 lb/gal HNO_3 × 1,000,000 gal solution/yr = 52 lb/yr

Example 4

A facility had an episodic release of nitric acid (HNO_3) in which the waste stream was temporarily below pH 6.0. During the episode, the waste water (pH 2.0) was discharged to a river for 20 minutes at a rate of 100 gallons per minute. Using Table 2-1, a pH of 2.0 for $HN0_3$ represents a concentration of 0.0052000 lb HNO_3/gallon of solution. The amount of the HNO_3 released can be estimated using the following equation:

Release of HNO_3 = (concentration of HNO_3) × (effluent flow rate).

Substituting the example values in the above equation:

Release of HNO_3 = 0.0052000 lb/gal × 100 gal/min × 20 min = 10 pounds

2.3.2 Estimating Treatment Efficiencies for Nitric Acid Neutralization

Nitric acid solutions that are neutralized to a pH of 6.0 or above have a treatment efficiency of 100 percent. If nitric acid is neutralized to a pH less than 6.0, then the reportable treatment efficiency is somewhere between 0 and 100 percent. It is possible to estimate the neutralization treatment efficiency using nitric acid concentration values directly from Table 2-1 in the equation given below. The concentrations correspond to the pH values before and after treatment.

Equation 1

Treatment Efficiency $(I-E)/I \times 100$

where

I = acid concentration before treatment
E = acid concentration after treatment

For strong acids only, including nitric acid, the net difference in pH before and after treatment can be used to estimate the treatment efficiency, since pH is directly proportional to the acid concentration. For example, a pH change of one unit results in a treatment efficiency of 90 percent, whether the pH change is from pH 1.0 to pH 2.0, or from pH 4.0 to pH 5.0.

Table 2-2 summarizes treatment efficiencies for various pH changes (the pH change is the difference between the initial pH and the pH after neutralization). In Table 2-2, some pH changes result in the same treatment efficiency values due to rounding to one decimal place.

Example 5

A nitric acid (HNO_3) waste stream of pH 2.4 is neutralized to pH 4.6. Using Table 2-1, the initial nitric acid concentration is 0.0021000 lb/gal and the final concentration is 0.0000130 lb/gal. Substituting these values into the equation for treatment efficiency:

Treatment Efficiency = (0.0021000 - 0.0000130)/0.0021000 × 100 = 99.4 percent.

Table 2-2: Nitric Acid Treatment Efficiencies for Various pH Changes

pH Change	Treatment Efficiency (%)
1.0	90.0
1.1	92.1
1.2	93.7
1.3	95.0
1.4	96.0
1.5	96.8
1.6	97.5
1.7	98.0
1.8	98.4
1.9	98.7
2.0	99.0
2.1	99.2
2.2	99.4
2.3	99.5
2.4	99.6
2.5	99.7
2.6	99.8
2.7	99.8
2.8	99.8
2.9	99.9
3.0	99.9

Example 6

If a nitric acid (HNO_3) waste stream of pH 2.0 is treated to pH 4.0, the pH change is 2 units. Using Table 2-2 above, the treatment efficiency is given as 99.0 percent.

2.3.3 Estimating Releases of Nitrate Compounds Generated from the Neutralization of Nitric Acid

The nitrate compounds produced from the complete neutralization (pH 6.0 or above) or partial neutralization (pH less than 6.0) of nitric acid are reportable under the nitrate compounds category if the appropriate threshold is met and should be included in all threshold and release calculations. In order to determine the quantity of a nitrate compound generated and released, the quantity of nitric acid released must be known (or calculated from the equations used in Examples 3 and 4 above) as well as the nitric acid treatment efficiency (calculated from the equations used in Examples 5 and 6 above).

The neutralization of nitric acid will most likely result in the generation of monovalent nitrate compounds (such as sodium nitrate and potassium nitrate). The quantity of these compounds formed in kilomoles will be equal to the quantity of the nitric acid neutralized in kilomoles. If divalent nitrate compounds are formed (such as calcium nitrate) the quantity of these compounds formed in kilomoles will be equal to one-half the quantity of the nitric acid neutralized in kilomoles. Similarly, if trivalent nitrate compounds are formed (such as iron (III) nitrate) the quantity formed of these compounds in kilomoles will be equal to one-third the quantity of the nitric acid neutralized in kilomoles. Note: To calculate the releases of nitrate compounds generated from the neutralization of nitric acid, the nitrate portion of molecular weight of the nitrate compound formed must be used. Molecular weights of some of the individual chemicals within the water dissociable nitrate compounds category are given in Table 3-1.

Example 7

In a calendar year, a facility transfers 50,000 pounds of nitric acid (HNO_3) to an on-site treatment facility. The nitric acid treatment efficiency is 95 percent, and the nitrate compound formed as a result of the treatment is sodium nitrate ($NaNO_3$). The quantity of nitric acid transferred that is neutralized (generating sodium nitrate) is 95 percent of 50,000 pounds, or 47,500 pounds. The molecular weight of nitric acid is 63.01 kg/kmol, and the molecular weight of sodium nitrate is 84.99 kg/kmol. The quantity of nitric acid neutralized is converted first to kilograms then to kilomoles using the following equations:

Kilograms HNO_3 neutralized = (lb HNO_3 neutralized) × (0.4536 kg/lb)
Kilomoles HNO_3 neutralized = (kg HNO_3) ÷ (MW of HNO_3 in kg/kmol)

Substituting the example values into the above equation yields:

Kilograms HNO_3 neutralized = 47,500 lb × 0.4536 kg/lb = 21,546 kg
Kilomoles HNO_3 neutralized = 21,546 kg ÷ 63.01 kg/kmol = 341.9 kmol

The quantity of sodium nitrate generated in kilomoles is equal to the quantity of nitric acid neutralized (341.9 kmol). The quantity of sodium nitrate generated in kilomoles is converted first to kilograms then to pounds using the following equations:

Kilograms $NaNO_3$ generated = (kmol $NaNO_3$) × (MW of $NaNO_3$ in kg/kmol)
Pounds $NaNO_3$ generated = (kg $NaNO_3$) × (2.205 lb/kg)

Substituting the values into the above equation yields:

Kilograms $NaNO_3$ generated = 341.9 kmol × 84.99 kg/kmol = 29,058 kg
Pounds $NaNO_3$ generated = 29,058 kg × 2.205 lb/kg = 64,073 pounds (reported as 64,000 pounds).

The 64,000 pounds of sodium nitrate generated is the quantity used to determine whether thresholds have been met or exceeded. The quantity of nitrate ion released is calculated as in Example 1 above.

Section 2.4 Generation of Nitrate Compounds from Biological Wastewater Treatment

If a facility treats wastewater on-site biologically, using the activated sludge process, for example, the facility may be generating nitrate compounds as by-products of this biological process. The nitrate ion generated from this process will be associated with various counterions (e.g. sodium ion, potassium ion). In the absence of information on the identity of the counterion, a facility should assume for the purposes of EPCRA section 313 threshold determinations that the counterion is sodium ion.

SECTION 3.0 CAS NUMBER LIST OF SOME OF THE INDIVIDUAL CHEMICALS WITHIN THE WATER DISSOCIABLE NITRATE COMPOUNDS CATEGORY

EPA is providing the following list of CAS numbers and chemical names to aid the regulated community in determining whether they need to report for the water dissociable nitrate compounds category. If a facility is manufacturing, processing, or otherwise using a chemical which is listed below, they must report this chemical. However, this list is not exhaustive. If a facility is manufacturing, processing, or otherwise using a water dissociable nitrate compound, they must report this chemical, even if it does not appear on the following list.

Table 3-1: Listing by CAS Number of Some of the Individual Chemicals within the Water Dissociable Nitrate Compounds Category

Chemical Name	Molecular Weight*	CAS Number
Aluminum nitrate, nonahydrate	213.00	7784-27-2
Ammonium nitrate	80.04	6484-52-2
Cerium (III) ammonium nitrate, tetrahydrate	486.22	13083-04-0
Cerium (IV) ammonium nitrate	548.23	10139-51-2
Barium nitrate	261.34	10022-31-8
Beryllium nitrate, trihydrate	133.02	7787-55-5
Cadmium nitrate	236.42	10325-94-7
Cadmium nitrate, tetrahydrate	236.42	10022-68-1
Calcium nitrate	164.09	10124-37-5
Calcium nitrate, tetrahydrate	164.09	13477-34-4
Cerium (III) nitrate, hexahydrate	326.13	10294-41-4
Cesium nitrate	194.91	7789-18-6
Chromium (III) nitrate, nonahydrate	238.01	7789-02-8
Cobalt (II) nitrate, hexahydrate	182.94	10026-22-9
Copper (II) nitrate, trihydrate	187.56	10031-43-3
Copper (II) nitrate, hexahydrate	187.56	13478-38-1
Dysprosium (III) nitrate, pentahydrate	348.51	10031-49-9
Erbium (III) nitrate, pentahydrate	353.27	10031-51-3
Gadolinium (III) nitrate, hexahydrate	343.26	19598-90-4
Gallium nitrate, hydrate	255.73	69365-72-6
Iron (III) nitrate, hexahydrate	241.86	13476-08-9
Iron (III) nitrate, nonahydrate	241.86	7782-61-8
Lanthanum (III) nitrate, hexahydrate	324.92	10277-43-7
Lead (II) nitrate	331.21	10099-74-8
Lithium nitrate	68.95	7790-69-4
Lithium nitrate, trihydrate	68.95	13453-76-4
Magnesium nitrate, dihydrate	148.31	15750-45-5
Magnesium nitrate, hexahydrate	148.31	13446-18-9

Chemical Name	Molecular Weight*	CAS Number
Manganese (II) nitrate, tetrahydrate	178.95	20694-39-7
Neodymium (III) nitrate, hexahydrate	330.25	16454-60-7
Nickel (II) nitrate, hexahydrate	182.70	13478-00-7
Potassium nitrate	101.10	7757-79-1
Rhodium (III) nitrate, dihydrate	288.92	13465-43-5
Rubidium nitrate	147.47	13126-12-0
Samarium (III) nitrate, hexahydrate	336.37	13759-83-6
Samarium (III) nitrate	230.97	13465-60-6
Samarium (III) nitrate, tetrahydrate	230.97	16999-44-3
Silver nitrate	169.87	7761-88-8
Sodium nitrate	84.99	7631-99-4
Strontium nitrate	211.63	10042-76-9
Strontium nitrate, tetrahydrate	211.63	13470-05-8
Terbium (III) nitrate, hexahydrate	344.94	13451-19-9
Thorium (IV) nitrate	480.06	13823-29-5
Thorium (IV) nitrate, tetrahydrate	480.06	13470-07-0
Yttrium (III) nitrate, hexahydrate	274.92	13494-98-9
Yttrium (III) nitrate, tetrahydrate	274.92	13773-69-8
Zinc nitrate, trihydrate	189.39	131446-84-9
Zinc nitrate, hexahydrate	189.39	10196-18-6
Zirconium (IV) nitrate, pentahydrate	339.24	13986-27-1

*For hydrated compounds, e.g. aluminum nitrate, nonahydrate, the molecular weight excludes the weight of the hydrate portion. For example, the same molecular weight is provided for aluminum nitrate, nonahydrate and aluminum nitrate.