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Project No. 112G00139

Mr. Howard Hickey
NAVFAC MW
201 Decatur Avenue
Building 1A, Code EV
Great Lakes, Illinois 60088

Reference: CLEAN Contract No. N62467-94-D-0888
Contract Task Order No. 0311, and

CLEAN Contract No. N62467-04-D-0055
Contract Task Order No. 0006

Subject: Monitoring for Degradation Products of Explosive Compounds
RDX, HMX, and TNT in Groundwater

Dear Mr. Hickey:

EPA has provided the following comments regarding monitoring of degradation products for explosives.

<u>SWMU 10 CMIP/QAPP E-Mail from Peter Ramanauskas (EPA Region 5) on November 2, 2006</u>:

Response to Comment 3: Monitored Natural Attenuation is the chosen remedy for this SWMU. We would like to discuss monitoring the primary contaminant breakdown products to fortify the evidence that RDX/TNT are degrading at this site. Based on the maximum RDX and TNT detections at Rockeye, could Tetra Tech provide the theoretical maximum values of degradation products which could potentially be generated and compare those to toxicological information/risk/based screening values and detection limits (based on the table provided in Attachment 1)? Even if the potential breakdown products would not be generated at levels that would be of health concern, the monitoring of a few intermediates will underscore whether the degradation process is progressing.

<u>SWMU 3 CMP for Ammunition Burning Grounds E-Mail from Peter Ramanauskas (EPA Region 5) on December 21, 2006</u>:

Response to Comment 17: (1) Section 2.6 should include a discussion of why the human health risks from incidental contact/ingestion of surface water are not an issue, (2) This section should be modified to include discussion of the complete explosive/organic breakdown products which could potentially be present in groundwater at MTA/OJT, (3) A discussion of the expected types and fate of explosives breakdown products for RDX, TNT, HMX which could be present in site groundwater and/or surface water should be presented. For example, the ATSDR Toxicity Profile for RDX identifies formaldehyde and nitrosamines as photoproducts identified from photolysis of RDX in aqueous solution; anaerobic biodegradation products included MNX, DNX, and TNS. Similarly, the ATSDR Toxicity Profiles identify a number of photodecomposition products for TNT and nitrate, nitrite, and formaldehyde for HMX; and (4) A study of the photolytic half-lives of RDX, HMX, and TNT in LSC surface waters would provide information how long the site contaminants would be expected to be present in surface water.

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The issue regarding explosive degradation products also applies to future CMPs and CMIP/QAPPs at SWMUs 12, 13, and 16.

An literature study has been conducted and various experts in the field have been contacted. The attached paper describes the study, the technical evaluations, and the resulting recommendations for monitoring of degradation products of explosives in groundwater and surface water.

Please contact me at (412) 921-8308 (email: Ralph.Basinski@ttnus.com) or Tom Johnston at (412) 921-8615 (email: Tom.Johnston@ttnus.com) regarding any questions or comments on the enclosed information.

Sincerely,

Ralph R. Basinski
Task Order Manager

RRB/mlg
Enclosure

cc: Mr. Tom Brent, NSWC Crane (letter and enclosure)
Ms. Debra Humbert, TtNUS, Inc. (letter only)
Mr. Mark Perry, TtNUS, Inc. (letter and enclosure)
Ms. Valerie Plachy, TtNUS, Inc. (letter and enclosure)
Dr. Tom Johnston, TtNUS, Inc. (letter and enclosure)
Mr. John Trepanowski, TtNUS, Inc. (letter and enclosure)
Mr. Garth Glenn, TtNUS, Inc. (letter only)
Ms. Lee Anne Rapp, NAVFAC Atlantic (PDF copy of letter via e-mail)
Ms. Bonnie Capito, NAVFAC Atlantic (PDF copy of letter via e-mail)
Mr. Ralph Basinski, TtNUS, Inc. (letter and enclosure)
File Copy – CTOs 0006, 0311, 0343, 0357, and 0377

WHITE PAPER:
MONITORING FOR DEGRADATION PRODUCTS OF EXPLOSIVE COMPOUNDS RDX, TNT, AND HMX IN GROUNDWATER NAVAL SURFACE WARFARE CENTER CRANE CRANE, INDIANA

1.0 BACKGROUND:

At the Naval Surface Warfare Center (NSWC) Crane located in Crane, Indiana, multiple Solid Waste Management Units (SWMUs) exhibit explosives contamination in groundwater and other environmental media (e.g., soil, surface water, sediment, and vegetation). The explosives detections are evidence of releases to these media, most which likely occurred as releases to soil with subsequent migration. Multiple environmental investigations have been conducted to establish the nature and extent of explosives contamination at individual SWMUs and the risks posed to humans and ecological receptors by contaminated environmental media.

The primary or parent explosive contaminants detected at NSWC Crane, include Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX), 2,4,6-Trinitrotouene (TNT), and octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) organic compounds. Of the explosives-related chemicals used in past operations and analyzed/detected in various environmental media at NSWC Crane, these three explosive compounds have the highest frequency of detection, the highest detected concentrations, or the highest number of environmental media detections at numerous SWMUs. Over time, these compounds have been shown by numerous researchers and practitioners to degrade naturally through biotic and abiotic processes into less complex compounds and ultimately convert to carbon dioxide, nitrogen, hydrogen, water, and other innocuous compounds. These naturally occurring degradation processes and other physical concentration reduction processes are described as natural attenuation.

United States Environmental Protection Agency (EPA) Region 5 has indicated a belief that some explosives degradation products may be toxic by themselves or may be even more toxic than the parent explosive compounds. The degradation of explosives may thus perpetuate or increase risks to human or ecological receptors until the generation of the non-toxic or significantly less toxic degradation products occurs. Currently, groundwater analysis for the primary parent explosive compounds (TNT, RDX, and HMX) and select degradation products occurs at several SWMUs at NSWC Crane where explosives are a contaminant of concern. EPA Region 5 has requested that NSWC Crane identify additional explosives-related degradation products for groundwater that are not currently being monitored at the facility. Additionally, EPA Region 5 has requested that any significantly toxic degradation products be included in groundwater monitoring programs at SWMUs where explosive contaminated groundwater exists.

2.0 OBJECTIVES:

The objectives of this white paper are to complete several tasks outlined by the EPA for NSWC Crane. These tasks in addition to other items that are necessary to achieve this request are as follows:

- Identify all degradation products formed upon the natural attenuation (e.g., degradation) of RDX, TNT, and HMX. This list shall include both those compounds currently being analyzed and those that are not being analyzed under current monitoring programs.

- Determine the potential for toxicity to human or ecological receptors for each of the explosives degradation products identified.

- Determine whether these compounds can currently be analyzed in commercial laboratories under approved methodologies (e.g., EPA methods).

- Based upon these findings determine whether analysis of these degradation compounds (including compounds currently being monitored and those that are not being monitored) is necessary to be protective of human health and the environment at NSWC Crane.

- Finally, based upon this analysis, make a recommendation to include the appropriate and required explosive compounds for sites at NSWC Crane that are currently being monitored for explosives compounds in groundwater.

3.0 APPROACH:

Because the degradation of explosive compounds is not as well understood as are other more common compounds (e.g., petroleum hydrocarbons, chlorinated solvents), a literature and information search was necessary to achieve the goals of this study. The four key steps necessary to address the EPA concern are as follows:

1. Identify and list known or potential RDX, TNT, and HMX degradation products. This list would be the compounds to be evaluated in this white paper.

2. Compile available chemical, physical, and toxicological data for the identified degradation products with the most toxic degradation compounds being of the greatest interest.

3. Identify current and potential analytical methods for quantifying the identified degradation products (i.e., the analytical methods used to quantify the degradation product concentrations in groundwater).

4. Utilize available explosives and degradation product analytical data for NSWC Crane groundwater with the information from Steps 1 through 3 to estimate the impact of each degradation product.

A literature search was conducted to gather information about the primary explosives (RDX, TNT, and HMX) and their known or potential degradation products. In addition, the following Tetra Tech, Inc. technical experts, were consulted: Rick Arnseth, Ronnie Britto, and Chris Pike. The information obtained from these experts was supplemented with information from a literature search. The literature search included publications from government and academic research papers to reviews of journal articles published by experts in the field of explosives degradation such as Jalal Hawari.

The three literature categories included literature:

1. From which information was extracted for this paper,

2. That was reviewed in detail but was not cited due to lack of information relevant to the purpose of this article, and

3. That was reviewed in a cursory manner and dismissed because it did not contain relevant information.

The first two categories are listed in the References section of this paper. The third category which included more than 5 times the number of technical journal articles, web links, and reports as the second category are not identified in this paper.

Based on the literature review, known or potential degradation products of each of the three primary explosives RDX, TNT, and HMX were identified for a variety of environmental conditions (see Section 4.0). Available chemical properties, physical properties, and toxicity data were then gathered for these explosives and the degradation products. In many cases, these data (i.e., chemical properties, physical properties, and toxicity data) for particular degradation chemicals could not be found. However, chemicals with similarity in chemical structure often have similar chemical or biochemical reactivity and hence similar toxicity. Therefore, if toxicity information was not available for a degradation chemical, a search was conducted to find a chemical with similar molecular structure (i.e., a search for a surrogate compound was conducted). When a surrogate compound was identified, the surrogate's toxicity data were used as an indirect indication of the toxicity for the target compound. In several cases, neither direct nor indirect toxicity data were available.

After identifying the likely or known degradation products, various commercial laboratories were contacted to determine the current and potential capabilities for analyzing RDX, TNT, and HMX degradation products that are identified in Section 4.0 is available.

An additional attempt was made to glean as much information as possible form available analytical data. Fundamental chemical data and available analytical data were also used, as appropriate, to make analytical methodology inferences. Many of the compounds of interest contain identical chemical functional groups such as nitro or nitroso groups. Ultraviolet-visible absorbance wavelengths for compounds with the same functional groups will not necessarily be identical but they will be similar. The spectroscopic absorption bands are characteristically broad because of interactions between the molecular energy levels of the chemicals and the solvent. It was noted that because of these similar absorption bands, past analytical results could contain evidence of the presence of other explosives-related degradation products even though the analytical systems were not calibrated for these additional chemicals. Many analyses for RDX, HMX, and TNT have been conducted in NSWC Crane groundwater using SW-846 Method 8330. This method employs reversed phase high performance liquid chromatography to separate the chemicals of interest. The chemicals are then quantified using ultraviolet absorption detection at a wavelength of 254 nanometers (nm). This wavelength is a commonly used "general purpose" wavelength for detecting organic compounds, especially for those compounds with double bonds in their chemical structures. Two different chromatograms are generated per sample. A review was conducted of the 60 chromatograms from analysis of 30 samples in sample delivery groups 27918 and 35724 collected in November 2003 and August 2005, respectively. These samples were collected from permanent groundwater wells across NSWC Crane. These samples were selected because they represented concentrations for RDX from non-detectable [about 0.25 micrograms per liter (µg/L) to the maximum observed concentration of 8,500 µg/L in sample 12GWT1604 for permanent groundwater wells.

The hypothesis underlying this chromatogram review was that a correlation between the presence and/or concentration of RDX and the appearance of minor chromatographic peaks that do not represent normal target analytes exists. If a correlation were detected, then a tentative conclusion that the extraneous peaks in the chromatographs represent degradation products for which the method is not normally calibrated is possible. Conversely, if such a correlation could not be identified or extraneous peaks were not present, it would <u>not</u> be proof that detectable levels of degradation products are not being generated, but, it would be cursory evidence that degradation products were not detectable by the routine explosives method. .

As a final step in the data review, ratios of parent compounds to daughter compounds (e.g., RDX to MNX, RDX to DNX, and RDX to TNX) concentrations were calculated from previous analytical data in an

attempt to evaluate the concentrations of subsequent degradation products. This is a somewhat subjective evaluation tool because kinetics data for degradation products are not available. Nevertheless, these ratios were thought to provide an indication of the maximum expected concentrations that are likely to be generated for degradation products from the primary compounds under typical groundwater conditions at NSWC Crane. These assumed maximum concentrations could then be used to estimate the possible contribution to risk for the degradation products.

4.0 FINDINGS

Tables 1 and 2 present the available data for various chemical and physical properties, as well as toxicity information, of potential explosives degradation products based on literature searches. In these tables, compounds are grouped to represent the parent explosives compounds and degradation products that are derived from the parents during degradation. Consequently, some compounds common to the degradation chain of more than one parent compound appear more than once in the tables. The following text presents a brief description of the primary degradation processes.

4.1 Degradation Pathways and Related Data

Multiple degradation pathways often exist for a chemical, each pathway owing its existence to a different set of environmental conditions. Degradation is often a sequential process in which one parent compound degrades into a daughter compound that in turn degrades into yet another compound, and so on until degradation is complete. Some conditions that affect the existence of these pathways and the degradation rates include concentrations of parent and daughter compounds, temperature, electron donor(s) present, species and concentrations of microorganisms present, concentrations of other chemical reactants, oxidation-reduction potential, and availability of light, pH, and ionic strength. Many explosive compounds can degrade under aerobic (i.e., in the presence of oxygen) or anaerobic (i.e., without oxygen) in microbial (biotic) and/or chemically mediated (abiotic) degradation.

The myriad of environmental conditions that exist confound the ability to predict precise degradation pathways of any chemical under particular conditions. Nevertheless, available studies generally agree with respect to the list of chemicals that are, or could be, produced from the degradation of RDX, TNT, and HMX. Therefore, it is likely that the chemicals identified to date as degradation products by various researchers represent the vast majority of compounds that would be produced during degradation of RDX, TNT, and HMX under a variety of conditions. These chemicals and associated chemical and physical properties are presented in Table 1. Degradation pathways thought to be the most probable or typical for RDX, TNT, and HMX are presented in Figures 1 through 3, respectively. Some of the chemicals listed in Table 1 have not been detected but were inferred from partial knowledge of the known degradation pathways. Nevertheless, they were included as potential targets for monitoring.

Another source of toxic chemicals other than RDX, TNT and HMX are chemicals that may be residual impurities from the manufacturing process. In RDX, for example, 1-acetylhexahydro-3,5-dinitro-1,3,5-triazine, is a known contaminant (ANRCP, 1998). A degradation product of this compound, methylene-N-(hydroxymethyl)-hydroxylamine-N'-(hydroxymethyl)-nitramine, was tentatively identified in ANRCP (1998) but was not shown to accumulate during RDX degradation. Contaminants of TNT include dinitrotoluenes. The list of chemicals in Table 1 includes two simple dinitrotoluenes and some dinitrotoluene derivatives. The literature generally shows that the degradation of HMX is similar to the degradation for RDX. Therefore, for this paper, it is presumed that impurities in HMX are also similar to impurities in RDX. Furthermore, HMX was detected considerably less frequently and at lower concentrations than RDX so minor components of HMX were considered not to be significant.

Table 2 presents toxicity data and risk-based screening values for the chemicals shown in Table 1. Where data were available, the screening values were based on direct toxicity data or on surrogate toxicity data. Sources of the data are identified in Table 2. Surrogate selection was based on similarity of chemical structure. In many cases, neither direct nor surrogate data could be found.

RDX is the most prevalent of the three parent compounds that are the subject of this paper. Drawing on research by others, Figure 2 shows one of the most prevalent likely degradation pathways for RDX under anaerobic conditions. The degradation pathways for TNT and HMX are most predominant under anaerobic conditions as are shown in Figures 2 and 3, respectively.

4.2 Qualitative Fate and Transport Model

RDX, TNT, HMX and other explosives at NSWC Crane were released directly to soil due to past operations. These chemicals leached from the soil via precipitation infiltration into the subsurface to the water table. Another transport pathway for these chemicals includes the precipitation flowing into surface drainage channels from where it migrates downstream. RDX and HMX do not exhibit strong adsorption to soils or stream sediments whereas TNT adsorbs more strongly to these environmental media. Therefore, RDX and HMX migrate readily into water whereas TNT migration is retarded by its propensity to adsorb to soil and bedrock. These explosives are subject to degradation in the presence of light (i.e., photolysis) and hydrolysis (i.e., reaction with water). Extremes of pH (i.e., high or low pH) can catalyze hydrolysis to accelerate the degradation. In groundwater, where light is not available and pH values are generally near neutral (i.e., pH = 7) at NSWC Crane, microbiological degradation, rather than abiotic degradation is more efficient and is the predominant degradation pathway. Microbial degradation can occur in either anaerobic or aerobic conditions and different products are formed under each set of conditions. Anaerobic degradation is considered to be the predominate mechanism for these explosive compounds, and the most studied.

A first step in the anaerobic microbiological degradation of RDX is the chemical reduction of a single nitro ($-NO_2$) functional group to a nitroso (-NO) group. The degradation pathway is shown in Figure 1. This type of reaction is fairly common in that nitro groups are commonly reduced to nitroso groups, amine groups ($-NH_2$), or hydroxylamine groups (-NHOH). The first mononitroso biodegradation product, MNX (hexahydro-1-nitroso-3,5-dinitro-1,3,5-triazine), can be broken down by two different pathways. In one pathway, a second nitro group is reduced to a nitroso group. This yields the dinitroso product, DNX (hexahydro-1,3-dinitroso-5-nitro-1,3,5-triazine). In the second pathway, the first nitroso group is reduced further to a hydroxylamine group to yield 1-hydroxylamino-3,5-dinitro-1,3,5-triazine. From this point, the number of pathways and products release increases rapidly, each time yielding a product of relatively equal complexity or yielding multiple products of lesser complexity. The researchers who first presented the degradation pathway displayed in Figure 1 observed an accumulation of mono-, di-, and tri-nitroso derivatives as the RDX disappeared. This observation, the decomposition of the MNX, and the detection of certain additional breakdown products, led the researchers to propose Figure 1 as a likely degradation scheme. However, it is likely that other degradation schemes or pathways exist for RDX. HMX degradation is generally considered to be similar to RDX degradation because of the chemical similarity between the two compounds, but HMX degradation has not been studied as thoroughly. TNT is not discussed in detail here and follows a different degradation scheme but the overall process (i.e., more parent compounds transforming into less complex daughter compounds) occurs. The TNT degradation products are shown in Tables 1 and 2.

The rate of transformation at each step of the degradation process is theoretically measurable; however, it often cannot be practically measured. A general principle of degradation is that a chemical will accumulate when its degradation rate is less than its production rate. Many degradation rates are sensitive to concentration so that the rate changes as the concentration of the chemical changes. These factors and their sensitivity to environmental conditions lead to inaccurate predictions for *in-situ* degradation rates. To facilitate the estimation of degradation rates, measurements are made under conditions that simplify the measurements and chemical degradation modeling is conducted using a mono-exponential decay. Mono-exponential decay dictates that chemical concentrations decrease exponentially. A characteristic of this decay is rapid concentration decrease at the beginning of degradation followed by increasingly slower rates of concentration decrease.

If a chemical follows a simple mono-exponential decay, it will have a characteristic half-life. Half-life is the time required to reduce the concentration of a chemical to half of its original concentration, regardless of initial concentration. This concept provides a convenient way to describe temporal changes in concentrations. For example, after 7 half-lives, the original concentration of a chemical will be less than one percent (i.e., $1/2^7 = 1/128^{th}$) of the concentration at the beginning of the decay period. The half-life is

an important environmental factor because it is an indication of the persistence of a chemical. Chemicals with long half-lives persist longer in the environment than chemicals with short half-lives. To put half-lives and their importance into perspective, consider the following. If the starting concentration of a chemical with half-life equal to 1 month in groundwater is 1,000 µg/L the chemical is not being replenished (i.e., source of the chemical no longer exists), the concentration at the end of the year would be about 0.24 µg/L.

The half-lives found for all identified degradation products of RDX, TNT, and HMX are presented in Table 1. For example, from Table 1 it is easy to derive the TNT half-life in anaerobic conditions as 1 to 12 months. This range of half-lives reflects the degree of uncertainty associated with these measurements. Also, evident in Table 1 is the dearth of half-life information. Half-life data is generally easily found in the literature for the three primary explosives (e.g., RDX, TNT, and HMX), however, the numerous daughter products are less studied and with few exceptions their half-lives were generally not found (Table 1). From these data, it is clear that TNT has the shortest photolytic half-life in surface water. RDX and HMX have approximately the same range of half-lives, which is about five times longer than the TNT half-life. The TNT groundwater half-life is considerably longer than TNT surface water half-life but RDX groundwater half-lives are about the same or less than the RDX surface water half-lives. Nitrite, nitrate, and formaldehyde were identified as photolytic degradation products of RDX and HMX (ANRCP, 1998).

The persistence of most of the chemicals in Tables 1 and 2 cannot be predicted because half-life data are not available.

4.3 Standard Analytical Methodologies

The primary explosives compounds (RDX, TNT, HMX and others) currently being analyzed are analyzed by a standardized method (SW-846 Method 8330). This method is used throughout the environmental industry and numerous environmental laboratories can perform the analysis. Several RDX and TNT degradation products have been analyzed at NSWC Crane in addition to the primary explosives. These compounds are: MNX, DNX, TNX, 2,2'-6,6'-tetranitro-4,4'-azoxytoluene, 2,4-diamino-6-nitrotoluene, 2,6-diam,ino-nitrotoluene, and 3,5-dinitroaniline. This second list of compounds cannot be analyzed directly by SW-846 Method 8330 so a modification of the method is used. Many of the remaining chemicals that are explosives degradation products are not currently analyzed and no standardized methods exist for their measurement. Analysis of these compounds would require a laboratory to develop and/or utilize unfamiliar analytical techniques. Under the best circumstances, existing methods can be used with little change to conduct non-standard chemical analyses. Under the worst circumstances, entirely new methods and analytical techniques would need to be developed to analyze non-standard chemicals. At the very least, quantification of any chemical requires the availability of a

standard on which the analytical system can be calibrated. In addition, the analytical method must be capable of quantifying the chemicals of interest at the concentrations of interest.

To determine what the current and potential future capabilities of environmental laboratories, eight commercial laboratories were polled. They were asked to indicate whether any of the chemicals listed in Tables 1 and 2 could be determined using existing, routine analytical methods. Only three laboratories responded. Table 3 displays the results of the poll. Very few of the chemicals were identified as being amenable to quantification by existing methods. The amenable chemicals were the 14 chemicals that appear on the SW-846 Method 8330 target analyte list. Only one of the laboratories can currently analyze the additional degradation products listed above but it is believed that other laboratories could also perform those analyses with minimal effort. The remaining seven laboratories were also polled to determine whether they thought existing analytical methods could be modified or new methods could be developed to quantify the compounds in Tables 1 and 2. Two laboratories responded, but neither of the laboratories indicated that minor or major method modifications or development would provide the capabilities to analyze for the remaining compounds in Tables 1 and 2.

A review of the National Environmental Methods Index (NEMI, http://www.nemi.gov/) revealed that standard analytical methods exist for formaldehyde, methanol, and 2-amino-nitrotoluene. The methods are identified later.

4.4 Toxicity

Preliminary remediation goals (PRGs) for most compounds in Table 2 are greater than the PRGs for RDX. PRGs are commonly used as the starting point for determining the concentrations to which a contaminated medium will be remediated. Actual cleanup goals may be significantly greater than the PRGs, depending on site-specific conditions and receptor pathways, but they are not often less than the PRGs. Chemicals with lower PRGs are generally more toxic than those with higher PRGs. PRGs presented in Table 2 are for human health risk effects. Also shown in Table 2 are ecological data screening levels. These levels also reflect the relative toxicities of chemicals, but to ecological receptors rather than human beings. Lower EDQLs reflect greater toxicity. In general, EDQLs are less than PRGs for at least one ecological receptor. Unfortunately, EDQLs are available only for chemicals commonly quantified using existing analytical methods.

4.5 Historical Laboratory Analyses

Table 4 shows that many chemical functional groups absorb ultraviolet light near a wavelength of 254 nm, including many of the functional groups associated with the explosives listed in Tables 1 and 2. In general, a wavelength less than about 220 nm or greater than about 285 nm would be expected to yield

only a weak absorbance at 254 nm unless the molar absorptivity is high. Several of the groups of interest or groups with similar structure to the groups of interest (i.e., amine, aldehyde, carboxyl, ester, nitrate, nitro, and nitrite) had relatively large molar absorptivities. This indicates that they should be detectable at 254 nm even though the sensitivities for these compounds might be less than for RDX, HMX, and TNT.

RDX was frequently the largest peak in chromatograms obtained from groundwater analyses using SW-846 Method 8330. In several cases, minor peaks were not visible or barely visible because the concentration scale was adjusted to ensure the largest peak was completely on scale. The associated quantitation report; however, provided peak area measurements that were useful for determining when a peak appeared at particular retention times as well as the relative size of the peak, even if it could not be seen on the chromatogram.

Based on visual inspection (i.e., statistical analyses were not performed) there appears to be no correlation between the number of unidentified peaks and the concentrations of RDX, HMX, or TNT. For example, when RDX concentrations were high, 10 or more small unidentified peaks may have been present and when RDX concentrations were low a similar number of small unidentified peaks were present. This correlation observation also holds true for HMX and TNT. Retention times or minor peaks did not appear to be correlated to the presence of RDX, HMX, or TNT although a rigorous review of was not performed. Minor peaks were not always present and their presence/absence was not correlated to explosives concentrations. This review did not provide a link between extraneous chromatographic peaks and the possible presence of degradation products that are not already included in the SW-846 Method 8330 analysis. The following possibilities remain:

- Additional degradation products were not present in the samples that were analyzed.
- Additional degradation products were present but are not detectable with SW-846 Method 8330.

4.6 Concentration Ratios for RDX and Primary Daughters.

Out of 853 RDX detections in groundwater samples at NSWC Crane groundwater, 90 samples had detectable levels of MNX, DNX, and/or TNX. The highest RDX degradation product concentrations were found where RDX concentrations were the highest. The most frequently detected of the primary RDX degradation products was MNX, the first product produced during chemical reduction of RDX. In the 86 samples in which RDX and MNX were both detected, the ratio of RDX concentration to MNX concentration was at least 3 to 1 (3:1) with a ratio of at least 11:1 in 84 of the samples. The maximum RDX:MNX ratio was 2,042:1. Hence, the concentration of MNX is typically less than one-tenth the RDX concentration and may be more than 2,000 times less than the RDX concentration.

In the 33 samples in which both RDX and DNX were detected, the minimum RDX:DNX concentration ratio was 3:1. Thirty out of the 33 samples had a ratio of at least 61:1. The maximum ratio was 5,122:1. Hence, the concentration of DNX is typically 50 times less than the RDX concentration and may be more than 5,000 times less.

In the 23 samples in which both RDX and TNX were detected, the minimum RDX:TNX concentration ratio was 52:1. All but three ratios were at least 152:1 and the maximum ratio was 9,730:1. Hence the TNX concentration is typically less than one one-hundredth the RDX concentration and may approach one ten-thousandth of the RDX concentration. The concentrations of subsequent degradation products are also likely to be very low, probably at least ten times less than the MNX, DNX, and TNX concentrations.

This observation is consistent with the inability to detect additional chromatographic peaks that are correlated with RDX, HMX, or TNT in the available data. It is acknowledged that this is not proof of the absence of the degradation products. However, if the concentration ratio of MNX to the next degradation product is comparable to the DNX concentration, the typical concentration for this daughter would be at least 50 times less than the RDX concentration. This means the maximum concentration of this chemical would be less than about 170 µg/L in any of the wells for which data are available. The actual concentration would probably be much less than 170 µg/L.

Based on the PRGs of Table 2 and the concentration ratios computed above, the toxicity presented by RDX degradation products that are more toxic than RDX would be of a magnitude similar to the RDX toxicity. For example, the groundwater PRG for hydroxymethyl-hydrazine (HMH) is 0.022 µg/L and the PRG for RDX is 0.61 µg/L (Table 2). This is a ratio of 0.61/0.022, or about 30:1. This means that 30 times less HMH than RDX would yield a toxicity equal to the RDX toxicity. If the HMH is assumed to be one-fiftieth the RDX concentration, the toxicity due to HMH would be approximately one-half the toxicity due to RDX. Based on the available data, most of the secondary degradation product concentrations are likely to be less than one-fiftieth the RDX concentration; and the secondary degradation product concentrations would contribute even less to the overall toxicity.

The observations described here are similar for HMX except that HMX is consistently detected less frequently and, when detected, is present is lower concentrations than RDX. For TNT, the degradation products are estimated to be less toxic than TNT, so the presence of secondary degradation products is of little concern.

5.0 CONCLUSIONS

Tables 1 and 2 are sparsely populated for lack of available data. Therefore, it is not possible to predict with any accuracy which of the likely or known degradation products of RDX, TNT, and HMX have a

significant chance of accumulating in the environment. Even if the secondary degradation product concentrations were known, the lack of toxicity data or risk-based concentrations levels for some of these compounds would render an accurate evaluation of their effect on receptors impossible. Nevertheless, the use of surrogate compounds did allow for estimating toxicities of several chemicals.

For groundwater, the PRG for TNT is at least one order of magnitude less than for the degradation products with available PRG data. Thus, TNT is the chemical of greatest concern in this degradation chain. The PRG for RDX, however, is greater than all of its degradation products shown in Table 2 except formaldehyde and methanol. Thus 1,1-dimethyl-hydrazine, 1,2-dimethyl-hydrazine, dimethyl-nitrosoamine, hydrazine, hydroxymethyl-hydrazine, and nitramide are of greater toxicological concern than RDX but formaldehyde and methanol are not. Unfortunately, the chemicals that are more toxic than RDX are not readily quantifiable due to a lack of published analytical methods for these chemical. HMX is similar to RDX in that the most toxic chemicals of the degradation chain, 1,1-dimethyl-hydrazine, hydrazine, and nitramide are not readily quantifiable by commonly used analytical methods. Lack of current analytical methods for the most toxic chemicals in the RDX and HMX degradation chains prevents the inclusion of those chemical in a monitoring program unless methods are modified or developed to quantify these chemicals.

The chromatogram review of available NSWC Crane groundwater analytical data did not yield a correlation that would indicate the presence of detectable levels of explosives degradation products other than those already included in the current analyses are present in the samples. This does not rule out the possibility that degradation products are present; it means that the routine analytical method appears to be unsuitable for identifying and quantifying these compounds.

One additional consideration is the relatively low contribution to risk from the more highly toxic degradation products. Although they are more toxic than the parent compounds, their expected concentrations are much less than the parents. Hence they do not significantly increase risk beyond that attributable to the parents ad primary degradation products. On this basis alone, the need to analyze for degradation products that are likely to be present in relatively low concentrations is questionable.

If chemical analyses for degradation products not already analyzed at NSWC Crane is necessary, specialty laboratories would need to be consulted/contracted. The laboratories would have to assess whether many of the identified degradation products could be quantified at concentrations of interest in groundwater. This will result in analytical costs that are considerably higher than normal analytical methods. Supposing that concentrations of all these chemicals could be quantified, many of these chemical only have limited toxicity data available to assess the associated risks. Fate and transport estimates would be limited because little or no fate and transport data could be found on the RDX, HMX,

and TNT degradation products, which is consistent with the information received from the technical experts (i.e., little information is available).

6.0 RECOMMENDATIONS

For routine groundwater monitoring purposes at NSWC Crane, the analysis of RDX, TNT, HMX, and the 11 other explosive compounds readily quantified with Method 8330 is recommended where groundwater is known to be or potentially contaminated with RDX, TNT or HMX. These compounds are:

- 1,3,5-trinitrobenzene
- 1,3-dinitrobenzene
- 2,4,6-trinitrotoluene (TNT)
- 2,4-dinitrotoluene
- 2,6-dinitrotoluene
- 2-amino-4,6-dinitrotoluene
- 2-nitrotoluene
- 3-nitrotoluene
- 4-amino-2,6-dinitrotoluene
- 4-nitrotoluene
- HMX
- nitrobenzene
- RDX
- tetryl

Analysis of the following additional degradation compounds in groundwater is recommended for consideration where RDX, TNT and HMX are known to be or are potential groundwater contaminants:

- MNX
- DNX
- TNX
- 2,2'-6,6'-tetranitro-4,4'-azoxytoluene
- 2,4-diamino-6-nitrotoluene
- 2,6-diam,ino-nitrotoluene
- 3,5-dinitroaniline

The likelihood of detecting these compounds, the cost of analysis, and the relative toxicities of these compounds should be considered.

Analysis of all other compounds identified in Tables 1 and 2 is not warranted, except perhaps in special circumstances, because the toxicities are not great enough to suggest that they present a significant risk to human receptors, or published analytical methods could not be found or too expensive to warrant their use given the low probability of detecting the compounds. Compounds for which methods could be found that fall into this category are:

- Formaldehyde
- 2-Amino-4-Nitrotoluene
- Methanol

Other methods may be available but it is more likely that existing methods would have to be modified or new methods developed to measure concentrations of any of the other degradation products at the concentrations that are expected in groundwater.

These recommendations are summarized in Table 5 for each compound.

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TABLE 1

RDX, TNT, HMX DEGRADATION PRODUCTS CHEMICAL AND PHYSICAL PROPERTIES

						Aerobic						Anaerobic						
						Biotic			Abiotic			Biotic						
Parent	Degradation Product	Abbr	CASRN	MW	Mol Formula	1/2 Life	Media	Mechanism	1/2 Life	Media	Mechanism	1/2 Life	Media	Mechanism	Solubility	Log K_{OW}	Source	Comments
NA	2,4,6-trinitrotoluene (TNT)	TNT	118-96-7	227.13	$C_7H_5N_3O_6$	1-6m	SW	microbial	14-84h	SW	photolysis	1-12m	GW	microbial	130	1.6, 2.2, 2.7, 1.84, 2.03, 3.2	1,2,3,7	
TNT	2-hydroxylamino-4,6-dinitrotoluene	2-HADNT	59283-76-0	213.15	$C_7H_7N_3O_5$	--	--	--	--	--	--	--	--	--	--	--	1	
TNT	4-hydroxylamino-2,6-dinitrotoluene	4-HADNT	59283-75-9	213.15	$C_7H_7N_3O_5$	--	--	--	--	--	--	--	--	--	--	--	1	
TNT	2-amino-4,6-dinitrotoluene	2-ADNT	35572-78-2	197	$C_7H_7N_3O_4$	--	--	--	--	--	--	--	--	--	38	1.95	1,2,5	
TNT	4-amino-2,6-dinitrotoluene	4-ADNT	19406-51-0	197	$C_7H_7N_3O_4$	--	--	--	--	--	--	--	--	--	43	1.9	1,2,5	
TNT	2,6-diamino-6-nitrotoluene	2,6-DANT		167.167	$C_7H_9N_3O_1$	--	--	--	--	--	--	--	--	--	--	--	1, 5	
TNT	2,4-diamino-6-nitrotoluene	2,4-DANT	6629-29-4	167.167	$C_7H_9N_3O_2$	--	--	--	--	--	--	--	--	--	--	--	1, 6	
TNT	2,4,6-triaminotoluene	TAT	634-87-7 (HCl)	137.184	$C_7H_{11}N_3$	--	--	--	--	--	--	--	soil	anaerobic only	--	--	1, 5	
TNT	2,2',4,4'-tetranitro-6,6'-azoxytoluene	--	--	407.28	$C_{14}H_{11}N_6O_9$	--	--	--	--	--	--	--	--	--	--	--	1	
TNT	2,2',4,6'-tetranitro-4,6'azoxytoluene	--	--	407.28	$C_{14}H_{11}N_6O_9$	--	--	--	--	--	--	--	--	--	--	--	1	
TNT	2,2',6,6'-tetranitro-4,4'azoxytoluene	--	--	407.28	$C_{14}H_{11}N_6O_9$	--	--	--	--	--	--	--	--	--	--	--	1	
TNT	1,3,5-trinitrobenzene	TNB	99-35-4	213.1062	$C_6H_3N_3O_6$	--	--	--	--	--	--	--	--	--	335	1.18	2	TNT photolysis
TNT	4,6-dinitroanthranil	--	--	206.124	$C_7H_3N_3O_5$	--	--	--	--	--	--	--	--	--	--	--	2	TNT photolysis
TNT	2,4,6-trinitrobenzaldehyde	--	606-34-8	241.1166	$C_7H_3N_3O_7$	--	--	--	--	--	--	--	--	--	--	--	2	TNT photolysis
TNT	2,4,6-trinitrobenzonitrile	--	--	238.12	$C_7H_2N_4O_6$	--	--	--	--	--	--	--	--	--	--	--	2	TNT photolysis
TNT	2,4-Dinitrotoluene	2,4-DNT	121-14-2	182.1354	$C_7H_6N_2O_4$	--	--	--	--	--	--	--	--	--	0.027 g/100 mL	--	11	TNT aerobic microbial
TNT	4-nitroso-2-nitrotoluene	--	--	166.138	$C_7H_6N_2O_3$	--	--	--	--	--	--	--	--	--	--	--	11	TNT aerobic microbial
TNT	2-nitroso-4-nitrotoluene	--	--	166.138	$C_7H_6N_2O_4$	--	--	--	--	--	--	--	--	--	--	--	11	TNT aerobic microbial
TNT	2-hydroxylamino-4-nitrotoluene	2HA-4NT	--	168.154	$C_7H_8N_2O_3$	--	--	--	--	--	--	--	--	--	--	--	11	TNT aerobic microbial
TNT	4-hydroxylamino-2-nitrotoluene	4HA-2NT	--	168.154	$C_7H_8N_2O_4$	--	--	--	--	--	--	--	--	--	--	--	11	TNT aerobic microbial
TNT	2-amino-4-nitrotoluene	2A-4NT	99-55-8	152.1524	$C_7H_8N_2O_2$	--	--	--	--	--	--	--	--	--	<0.1 g/100 mL	--	11	TNT aerobic microbial
TNT	4-amino-2-nitrotoluene	4A-2NT	119-32-4	152.1524	$C_7H_8N_2O_2$	--	--	--	--	--	--	--	--	--	<0.1 g/100 mL	--	11	TNT aerobic microbial
TNT	2,4-diaminonitrotoluene	2,4-DAT	--	167.167	$C_7H_9N_3O_2$	--	--	--	--	--	--	--	--	--	--	--	11	TNT aerobic microbial
TNT	4,2'-dinitro-2,6'azoxytoluene	--	--	343.288	$C_{14}H_{11}N_6O_5$	--	--	--	--	--	--	--	--	--	--	--	11	TNT aerobic microbial
TNT	2,6-Dinitrotoluene	2,6-DNT	606-20-2	182.1354	$C_7H_6N_2O_4$	--	--	--	--	--	--	--	--	--	0.0182 g/100 mL	--	11	TNT aerobic microbial
TNT	2-amino-6-nitrotoluene	2A-6NT	603-83-8	152.1524	$C_7H_8N_2O_2$	--	--	--	--	--	--	--	--	--	<0.1 g/100 mL	--	11	TNT aerobic microbial
TNT	2,6-diaminonitrotoluene	2,6-DAT	--	167.167	$C_7H_9N_3O_1$	--	--	--	--	--	--	--	--	--	--	--	11	TNT aerobic microbial
TNT	2,6-diamino-4-nitrotoluene	--	--	167.167	$C_7H_9N_3O_1$	--	--	--	--	--	--	--	--	--	--	--		
TNT	2,4,6-trinitrobenzylalcohol	--	--	243.13	$C_7H_5N_3O_7$	--	--	--	--	--	--	--	--	--	--	--	7	
TNT	trinitrobenzoic acid	TNBA	129-66-8	257.116	$C_7H_3N_3O_8$	--	--	--	--	--	--	--	--	--	--	--	7	
TNT	4-amino-2,6-dinitrobenzylalcohol	--	--	213.156	$C_7H_7N_3O_5$	--	--	--	--	--	--	--	--	--	--	--	7	
TNT	2,4-diamino-6-nitrobenzylalcohol	--	--	183.172	$C_7H_9N_3O_3$	--	--	--	--	--	--	--	--	--	--	--	7	
TNT	2,4-diamino-6-nitrobenzoic acid	--	--	211.156	$C_7H_7N_3O_4$	--	--	--	--	--	--	--	--	--	--	--	7	
TNT	5-nitro-*m*-phenylenediamine	--	5042-55-7	153.1402	$C_6H_7N_3O_2$	--	--	--	--	--	--	--	--	--	--	--	7	
TNT	4-amino-2,6-dinitro-*m*-cresol	--	--	213	$C_7H_7N_3O_5$	--	--	--	--	--	--	--	--	--	--	--	7	
NA	hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX)	RDX	121-82-4	222.26	$C_3H_6N_6O_6$	4d (sludge)	--	--	0.7-15d	SW	photolysis	--	--	--	42.3	0.87	1,3,5,10,12	
RDX	hexahydro-1,3,5-mononitroso-1,3,5-triazine	MNX	--	206.26	$C_3H_6N_6O_5$	--	--	--	--	--	--	--	--	--	--	--	1,10	
RDX	hexahydro-1,3,5-dinitroso-1,3,5-triazine	DNX	--	190.26	$C_3H_6N_6O_4$	--	--	--	--	--	--	--	--	--	--	--	1,10	
RDX	hexahydro-1,3,5-trinitroso-1,3,5-triazine	TNX	13980-04-6	174.1188	$C_3H_6N_6O_3$	--	--	--	--	--	--	--	--	--	--	--	1,10	
RDX	1-hydroxylamino-3,5-dinitro-1,3,5-triazine	--	--	208.276	$C_3H_8N_6O_5$	--	--	--	--	--	--	--	--	--	--	--	1,10	
RDX	1-hydroxylamino-3-nitroso-5-nitro-1,3,5-triazine	--	--	192.276	$C_3H_8N_6O_4$	--	--	--	--	--	--	--	--	--	--	--	1,10	
RDX	1-hydroxylamino-3,5-dinitroso-1,3,5-nitro-1,3,5-triazine	--	--	174.1188	$C_3H_8N_6O_3$	--	--	--	--	--	--	--	--	--	--	--	1,10	
RDX	N-hydroxy-methylethylene-dinitramine	--	--	166.108	$C_2H_6N_4O_5$	--	--	--	--	--	--	--	--	--	--	--	1,10	
RDX	N-hydroxyl-amino-N'-nitro-methylenediamine	--	--	122.098	$CH_6N_4O_3$	--	--	--	--	--	--	--	--	--	--	--	4,10	
RDX	N-hydroxyl-amino-N'-nitroso-methylenediamine	--	--	106.098	$CH_6N_4O_2$	--	--	--	--	--	--	--	--	--	--	--	4,10	
RDX	N-hydroxyl-methylene hydrazone	--	--	60.062	CH_4N_2O	--	--	--	--	--	--	--	--	--	--	--	4,10	
RDX	methylene-dinitramine	--	--	136.082	$CH_4N_4O_4$	--	--	--	--	--	--	--	--	--	--	--	4,10	
RDX	nitramide	--	7782-94-7	62.028	$H_2N_2O_2$	--	--	--	--	--	--	--	--	--	--	--	4,10	
RDX	hydroxymethyl-hydrazine	--	--	62.078	CH_6N_2O	--	--	--	--	--	--	--	--	--	--	--	4,10	
RDX	dimethyl-nitrosoamine	--	62-75-9	74.0822	$C_2H_6N_2O$	--	--	--	--	--	--	--	--	--	10g/100mL	--	4,10	

TABLE 1

RDX, TNT, HMX DEGRADATION PRODUCTS CHEMICAL AND PHYSICAL PROPERTIES

						Aerobic						Anaerobic						
						Biotic			Abiotic			Biotic						
Parent	Degradation Product	Abbr	CASRN	MW	Mol Formula	1/2 Life	Media	Mechanism	1/2 Life	Media	Mechanism	1/2 Life	Media	Mechanism	Solubility	Log K_{OW}	Source	Comments
RDX	hydrazine	--	302-01-2	32.045	H_4N_2	--	--	--	--	--	--	--	--	--	miscible	--	1,10	
RDX	1,1-dimethyl-hydrazine	--	57-14-7	60.1	$C_2H_8N_2$	--	--	--	--	--	--	--	--	--	miscible	-1.19	1,10	
RDX	1,2-dimethyl-hydrazine	--	540-73-8	60.1	$C_2H_8N_2$	--	--	--	--	--	--	--	--	--	miscible	-0.54	1,10	
RDX	formaldehyde	--	50-00-0	30.0262	CH_2O	--	--	--	--	--	--	--	--	--	55g/100mL	--	1,10	
RDX	methanol	--	--	32.042	CH_4O	--	--	--	--	--	--	--	--	--	--	--	1,10	
RDX	4,6-dinitro-4,6-diaza-hexanal	--	--	193.136	$C_3H_7N_5O_5$	--	--	--	--	--	--	--	--	--	--	--	9	
RDX	5-hydroxy-4-nitro-2,4-diaza-pentanal	--	--	149.116	$C_3H_7N_3O_4$	--	--	--	--	--	--	--	--	--	--	--	9	
RDX	4-nitro-2,4-diaza-butanal	4-NDAB	--	119.09	$C_2H_5N_3O_3$	--	--	--	--	--	--	--	--	--	--	--	9	
NA	octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX)	HMX	2691-41-0	296.2	$C_4H_8N_8O_8$	17h	--	--	2-17d	SW	photolysis	--	--	--	6.6	0.26, 0.13, 0.06	1,3,5,12	
HMX	octahydro-1-nitroso-3,5,7-trinitro-1,3,5,7-tetrazocine	mNs-HMX	--	280.2	$C_4H_8N_8O_7$	--	--	--	--	--	--	--	--	--	--	--	3,8	
HMX	octahydro-1,3-dinitroso-5,7-dinitro-1,3,5,7-tetrazocine	aNs-HMX	--	264.2	$C_4H_8N_8O_6$	--	--	--	--	--	--	--	--	--	--	--	3	
HMX	octahydro-1,5-dinitroso-3,7-dinitro-1,3,5,7-tetrazocine	--	--	264.2	$C_4H_8N_8O_6$	--	--	--	--	--	--	--	--	--	--	--	10	
HMX	octahydro-1,3,5-trinitroso-7-nitro-1,3,5,7-tetrazocine	--	--	248.2	$C_4H_8N_8O_5$	--	--	--	--	--	--	--	--	--	--	--	3	
HMX	octahydro-1,3,5,7-tetranitroso-1,3,5,7-tetrazocine	--	--	232.2	$C_4H_8N_8O_4$	--	--	--	--	--	--	--	--	--	--	--	3	
HMX	bis(hydroxymethyl)nitramine	--	--	122.088	$C_2H_6N_2O_4$	--	--	--	--	--	--	--	--	--	--	--	4	
HMX	N-hydroxy-methylethylene-dinitramine	--	--	166.108	$C_2H_6N_4O_5$	--	--	--	--	--	--	--	--	--	--	--	4	
HMX	methylene-dinitramine	--	--	136.082	$CH_4N_4O_4$	--	--	--	--	--	--	--	--	--	--	--	4	
HMX	nitramide	--	7782-94-7	62.028	$H_2N_2O_2$	--	--	--	--	--	--	--	--	--	--	--	4	
HMX	hydrazine	--	302-01-2	32.045	H_4N_2	--	--	--	--	--	--	--	--	--	miscible	--	4	
HMX	1,1-dimethyl-hydrazine	--	57-14-7	60.1	$C_2H_8N_2$	--	--	--	--	--	--	--	--	--	miscible	-1.19	4	
HMX	formaldehyde	--	50-00-0	30.0262	CH_2O	--	--	--	--	--	--	--	--	--	55g/100mL	--	4	
HMX	methanol	--	50-00-0	32.042	CH_2O	--	--	--	--	--	--	--	--	--	--	--	4	
HMX	4-nitro-2,4-diaza-butanal	4-NDAB	--	119.09	$C_2H_5N_3O_3$	--	--	--	--	--	--	--	--	--	--	--	9	

References

1 Talmage, et al. 1999
2 Major et al., 2002
3 Monteil-Riviera et al. 2003
4 Hawari et al. 2001;
5 Sunhara et al. 1998
6 Sunhara et al. 2001
7 ATSDR , 1995a
8 ATSDR , 1995b
9 Balakrishnan et al., 2002
10 Card and Autenrieth, 1998
11 Dodard, et al., 1999
12 ANRCP, 1998

Notes:

No anaerobic abiotic half-lives were found for any of the compounds in this table.
ATSDR = Agency for Toxic Substances and Disease Registry
-- Intentionally left blank because information was not found.

Abbreviations:

Abbr	Abbreviation
CASRN	Chemical Abstracts Service Registry Number
Kow	Octanol-water partition coefficient
Mol	Molecular
MW	Molecular Weight

TABLE 2

RDX, TNT, HMX DEGRADATION PRODUCTS AND TOXICITY DATA

						Region 9 PRGs			Ecological Receptors						Toxicity				
						Soil	Water		Surface Water	Sediment	Surface soil				Microtox		Algal		
Parent	Degradation Product	Abbr	CASRN	MW.	Mol Formula	mg/kg	µg/L	Comments	(mg/L)	(mg/kg)	Plants (mg/kg)	Invertebrates (mg/kg)	Wildlife (mg/kg)	BCF	IC50	IC20	EC50	EC20	References
NA	2,4,6-trinitrotoluene (TNT)	TNT	118-96-7	227.13	$C_7H_5N_3O_6$	16	2.2	–	0.09	0.09[1]	30	140	–	209-DM	3.4	0.2	2.5	1.9	1,2,3,7
TNT	2-hydroxylamino-4,6-dinitrotoluene	2-HADNT	59283-76-0	213.15	$C_7H_7N_3O_5$	120	73	–	–	–	–	–	–	–	–	–	–	–	1
TNT	4-hydroxylamino-2,6-dinitrotoluene	4-HADNT	59283-75-9	213.15	$C_7H_7N_3O_5$	120	73	–	–	–	–	–	–	–	–	–	–	–	1
TNT	2-amino-4,6-dinitrotoluene	2-ADNT	35572-78-2	197	$C_7H_7N_3O_4$	120	73	–	0.02	–	80	–	–	–	>112.6	95.8	–	–	1,2,5
TNT	4-amino-2,6-dinitrotoluene	4-ADNT	19406-51-0	197	$C_7H_7N_3O_4$	120	73	–	–	–	–	–	–	–	>131.2	45.7	–	–	1,2,5
TNT	2,6-diamino-6-nitrotoluene	2,6-DANT		167.167	$C_7H_9N_3O_1$	120	73	–	–	–	–	–	–	–	>306.4	137.7	–	–	1, 5
TNT	2,4-diamino-6-nitrotoluene	2,4-DANT	6629-29-4	167.167	$C_7H_9N_3O_2$	120	73	–	–	–	–	–	–	–	–	119	–	–	1, 6
TNT	2,4,6-triaminotoluene	TAT	634-87-7 (HCl)	137.184	$C_7H_{11}N_3$	31	18	–	–	–	–	–	–	–	>188.2	171.6	–	–	1, 5
TNT	2,2',4,4'-tetranitro-6,6'-azoxytoluene	–	–	407.28	$C_{14}H_{11}N_6O_9$	31	18	–	–	–	–	–	–	–	–	–	–	–	1
TNT	2,2',4,6'-tetranitro-4,6'azoxytoluene	–	–	407.28	$C_{14}H_{11}N_6O_9$	31	18	–	–	–	–	–	–	–	–	–	–	–	1
TNT	2,2',6,6'-tetranitro-4,4'azoxytoluene	–	–	407.28	$C_{14}H_{11}N_6O_9$	31	18	–	–	–	–	–	–	–	–	–	–	–	1
TNT	1,3,5-trinitrobenzene	TNB	99-35-4	213.1062	$C_6H_3N_3O_6$	1800	1100	–	0.011	0.002[1]	–	–	–	–	–	–	–	–	2
TNT	4,6-dinitroanthranil	–	–	206.124	$C_7H_3N_3O_5$	NA	NA	–	–	–	–	–	–	–	–	–	–	–	2
TNT	2,4,6-trinitrobenzaldehyde	–	606-34-8	241.1166	$C_7H_3N_3O_7$	NA	NA	–	–	–	–	–	–	–	–	–	–	–	2
TNT	2,4,6-trinitrobenzonitrile	–	–	238.12	$C_7H_2N_4O_6$	NA	NA	–	–	–	–	–	–	–	–	–	–	–	2
TNT	2,4-Dinitrotoluene	2,4-DNT	121-14-2	182.1354	$C_7H_6N_2O_4$	120	73	–	0.31	0.0144[2]	–	–	–	–	269	44.1	–	–	11
TNT	4-nitroso-2-nitrotoluene	–	82414-03-7	166.138	$C_7H_6N_2O_3$	120	73	–	–	–	–	–	–	–	–	–	–	–	11
TNT	2-nitroso-4-nitrotoluene	–	–	166.138	$C_7H_6N_2O_4$	120	73	–	–	–	–	–	–	–	–	–	–	–	11
TNT	2-hydroxylamino-4-nitrotoluene	2HA-4NT	–	168.154	$C_7H_8N_2O_3$	120	73	–	–	–	–	–	–	–	–	–	–	–	11
TNT	4-hydroxylamino-2-nitrotoluene	4HA-2NT	–	168.154	$C_7H_8N_2O_4$	120	73	–	–	–	–	–	–	–	–	–	–	–	11
TNT	2-amino-4-nitrotoluene	2A-4NT	99-55-8	152.1524	$C_7H_8N_2O_2$	120	73	–	–	–	–	–	–	–	94.3	30.2	–	–	11
TNT	4-amino-2-nitrotoluene	4A-2NT	119-32-4	152.1524	$C_7H_8N_2O_2$	120	73	–	–	–	–	–	–	–	43.5	13.1	–	–	11
TNT	2,4-diaminonitrotoluene	2,4-DAT	–	167.167	$C_7H_9N_3O_2$	120	73	–	–	–	–	–	–	–	405.7	102.3	–	–	11
TNT	4,2'-dinitro-2,6'azoxytoluene	–	–	343.288	$C_{14}H_{11}N_6O_5$	31	18	–	–	–	–	–	–	–	–	–	–	–	11
TNT	2,6-Dinitrotoluene	2,6-DNT	606-20-2	182.1354	$C_7H_6N_2O_4$	61	36	–	–	0.0398[2]	–	–	–	–	16.4	4.2	–	–	11
TNT	2-amino-6-nitrotoluene	2A-6NT	603-83-8	152.1524	$C_7H_8N_2O_2$	61	36	–	–	–	–	–	–	–	22.8	5.3	–	–	11
TNT	2,6-diaminonitrotoluene	2,6-DAT	–	167.167	$C_7H_9N_3O_1$	61	36	–	–	–	–	–	–	–	>608.8	597.4	–	–	11
TNT	2,6-diamino-4-nitrotoluene	–	–	167.167	$C_7H_9N_3O_1$	–	–	–	–	–	–	–	–	–	–	–	–	–	
TNT	2,4,6-trinitrobenzylalcohol	–	–	243.13	$C_7H_5N_3O_7$	–	–	–	–	–	–	–	–	–	–	–	–	–	7
TNT	trinitrobenzoic acid	TNBA	129-66-8	257.116	$C_7H_3N_3O_8$	–	–	–	–	–	–	–	–	–	–	–	–	–	7
TNT	4-amino-2,6-dinitrobenzylalcohol	–	–	213.156	$C_7H_7N_3O_5$	–	–	–	–	–	–	–	–	–	–	–	–	–	7
TNT	2,4-diamino-6-nitrobenzylalcohol	–	–	183.172	$C_7H_9N_3O_3$	–	–	–	–	–	–	–	–	–	–	–	–	–	7
TNT	2,4-diamino-6-nitrobenzoic acid	–	–	211.156	$C_7H_7N_3O_4$	–	–	–	–	–	–	–	–	–	–	–	–	–	7
TNT	5-nitro-*m*-phenylenediamine	–	5042-55-7	153.1402	$C_6H_7N_3O_2$	1800	1100	–	–	–	–	–	–	–	–	–	–	–	7
TNT	4-amino-2,6-dinitro-*m*-cresol	–	–	213	$C_7H_7N_3O_5$	–	–	–	–	–	–	–	–	–	–	–	–	–	7
NA	hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX)	RDX	121-82-4	222.26	$C_3H_6N_6O_6$	4.4	0.61	as total RDX (3)	0.19	0.01[1]	100	–	–	5-FHM	>181	104.6	–	–	1,3,5,10
RDX	hexahydro-1,3,5-mononitroso-1,3,5-triazine	MNX	–	206.26	$C_3H_6N_6O_5$	4.4	0.61	as total RDX (3)	–	–	–	–	–	–	–	–	–	–	1,10
RDX	hexahydro-1,3,5-dinitroso-1,3,5-triazine	DNX	–	190.26	$C_3H_6N_6O_4$	4.4	0.61	as total RDX (3)	–	–	–	–	–	–	–	–	–	–	1,10
RDX	hexahydro-1,3,5-trinitroso-1,3,5-triazine	TNX	13980-04-6	174.1188	$C_3H_6N_6O_3$	4.4	0.61	as total RDX (3)	–	–	–	–	–	–	–	–	–	–	1,10
RDX	1-hydroxylamino-3,5-dinitro-1,3,5-triazine	–	–	208.276	$C_3H_8N_6O_5$	4.4	0.61	as total RDX (3)	–	–	–	–	–	–	–	–	–	–	1,10
RDX	1-hydroxylamino-3-nitroso-5-nitro-1,3,5-triazine	–	–	192.276	$C_3H_8N_6O_4$	4.4	0.61	as total RDX (3)	–	–	–	–	–	–	–	–	–	–	1,10
RDX	1-hydroxylamino-3,5-dinitroso-1,3,5-nitro-1,3,5-triazine	–	–	174.1188	$C_3H_8N_6O_3$	4.4	0.61	as total RDX (3)	–	–	–	–	–	–	–	–	–	–	1,10
RDX	N-hydroxy-methylethylene-dinitramine	–	–	166.108	$C_2H_6N_4O_5$	NA	NA	–	–	–	–	–	–	–	–	–	–	–	1,10
RDX	N-hydroxyl-amino-N'-nitro-methylenediamine	–	–	122.098	$CH_6N_4O_3$	NA	NA	–	–	–	–	–	–	–	–	–	–	–	4,10
RDX	N-hydroxyl-amino-N'-nitroso-methylenediamine	–	–	106.098	$CH_6N_4O_2$	NA	NA	–	–	–	–	–	–	–	–	–	–	–	4,10
RDX	N-hydroxyl-methylene hydrazone	–	–	60.062	CH_4N_2O	NA	NA	–	–	–	–	–	–	–	–	–	–	–	4,10
RDX	methylene-dinitramine	–	–	136.082	$CH_4N_4O_4$	NA	NA	–	–	–	–	–	–	–	–	–	–	–	4,10
RDX	nitramide	–	7782-94-7	62.028	$H_2N_2O_2$	NA	NA	–	–	–	–	–	–	–	–	–	–	–	4,10
RDX	hydroxymethyl-hydrazine	–	–	62.078	CH_6N_2O	0.16	0.022	–	–	–	–	–	–	–	–	–	–	–	4,10
RDX	dimethyl-nitrosoamine	–	62-75-9	74.0822	$C_2H_6N_2O$	0.0013	0.013	–	–	–	–	–	–	–	–	–	–	–	4,10
RDX	hydrazine	–	302-01-2	32.045	H_4N_2	0.16	0.022	–	–	–	–	–	–	–	–	–	–	–	1,10
RDX	1,1-dimethyl-hydrazine	–	57-14-7	60.1	$C_2H_8N_2$	0.16	0.022	–	–	–	–	–	–	–	–	–	–	–	1,10
RDX	1,2-dimethyl-hydrazine	–	540-73-8	60.1	$C_2H_8N_2$	0.16	0.022	–	–	–	–	–	–	–	–	–	–	–	1,10
RDX	formaldehyde	–	50-00-0	30.0262	CH_2O	9200	5500	–	–	–	–	–	–	–	–	–	–	–	1,10
RDX	methanol	–	–	32.042	CH_4O	31000	18000	–	–	–	–	–	–	–	–	–	–	–	1,10

TABLE 2

RDX, TNT, HMX DEGRADATION PRODUCTS AND TOXICITY DATA

						Region 9 PRGs			Ecological Receptors						Toxicity				
						Soil	Water		Surface Water	Sediment	Surface soil				Microtox		Algal		
Parent	Degradation Product	Abbr	CASRN	MW	Mol Formula	mg/kg	µg/L	Comments	(mg/L)	(mg/kg)	Plants (mg/kg)	Invertebrates (mg/kg)	Wildlife (mg/kg)	BCF	IC50	IC20	EC50	EC20	References
RDX	4,6-dinitro-4,6-diaza-hexanal	–	–	193.136	$C_3H_7N_5O_5$	–	–	–	–	–	–	–	–	–	–	–	–	–	9
RDX	5-hydroxy-4-nitro-2,4-diaza-pentanal	–	–	149.116	$C_3H_7N_3O_4$	–	–	–	–	–	–	–	–	–	–	–	–	–	9
RDX	4-nitro-2,4-diaza-butanal	4-NDAB		119.09	$C_2H_5N_3O_3$	–	–	–	–	–	–	–	–	–	–	–	–	–	9
NA	octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX)	HMX	2691-41-0	296.2	$C_4H_8N_8O_8$	3100	1800	as total HMX (3)	0.33	0.005[1]	–	–	–	–	>21.7	>21.8	–	–	1,3,5
HMX	octahydro-1-nitroso-3,5,7-trinitro-1,3,5,7-tetrazocine	mNs-HMX	–	280.2	$C_4H_8N_8O_7$	3100	1800	as total HMX (3)	–	–	–	–	–	–	–	–	–	–	3,8
HMX	octahydro-1,3-dinitroso-5,7-dinitro-1,3,5,7-tetrazocine	–	–	264.2	$C_4H_8N_8O_6$	3100	1800	as total HMX (3)	–	–	–	–	–	–	–	–	–	–	
HMX	octahydro-1,5-dinitroso-3,7-dinitro-1,3,5,7-tetrazocine	dNs-HMX	–	264.2	$C_4H_8N_8O_6$	3100	1800	as total HMX (3)	–	–	–	–	–	–	–	–	–	–	3
HMX	octahydro-1,3,5-trinitroso-7-nitro-1,3,5,7-tetrazocine	–	–	248.2	$C_4H_8N_8O_5$	3100	1800	as total HMX (3)	–	–	–	–	–	–	–	–	–	–	3
HMX	octahydro-1,3,5,7-tetranitroso-1,3,5,7-tetrazocine	–	–	232.2	$C_4H_8N_8O_4$	3100	1800	as total HMX (3)	–	–	–	–	–	–	–	–	–	–	3
HMX	bis(hydroxymethyl)nitramine	–	–	122.088	$C_2H_6N_2O_4$	NA	NA	–	–	–	–	–	–	–	–	–	–	–	4
HMX	N-hydroxy-methylethylene-dinitramine	–	–	166.108	$C_2H_6N_4O_5$	NA	NA	–	–	–	–	–	–	–	–	–	–	–	4
HMX	methylene-dinitramine	–	–	136.082	$CH_4N_4O_4$	NA	NA	–	–	–	–	–	–	–	–	–	–	–	4
HMX	nitramide	–	7782-94-7	62.028	$H_2N_2O_2$	0.16	0.022	–	–	–	–	–	–	–	–	–	–	–	4
HMX	hydrazine	–	302-01-2	32.045	H_4N_2	0.16	0.022	–	–	–	–	–	–	–	–	–	–	–	4
HMX	1,1-dimethyl-hydrazine	–	57-14-7	60.1	$C_2H_8N_2$	0.16	0.022	–	–	–	–	–	–	–	–	–	–	–	4
HMX	formaldehyde	–	50-00-0	30.0262	CH_2O	9200	5500	–	–	–	–	–	–	–	–	–	–	–	4
HMX	methanol	–	–	32.042	CH_4O	31000	18000	–	–	–	–	–	–	–	–	–	–	–	4
HMX	4-nitro-2,4-diaza-butanal	4-NDAB	–	119.09	$C_2H_5N_3O_3$	–	–	–	–	–	–	–	–	–	–	–	–	–	9

References:

1 Talmage, et al. 1999
2 Major et al., 2002
3 Monteil-Riviera et al. 2003
4 Hawari et al. 2001;
5 Sunhara et al. 1998
6 Sunhara et al. 2001
7 ATSDR , 1995a
8 ATSDR , 1995b
9 Balakrishnan et al., 2002
10 Card and Autenrieth, 1998
11 Dodard, et al., 1999

Abbreviation:

µg/kg	Microgram per kilogram
Abbr	Abbreviation
ATSDR	Agency for Toxic Substances and Disease Registry
BCF	Bioconcentration factor
CASRN	Chemical Abstracts Service Registry Number
DM	*Daphnia magna*
EC20	Effect Concentration 20
EC50	Effect Concentration 50
FHM	Fat Head Minnow
IC20	Inhibition Concentration 20
IC50	Inhibition Concentration 50
mg/kg	Milligram per kilogram
Mol	Molecular
MW	Molecular Weight
PRG	Preliminary Remediation Goal
–	Intentionally left blank because information was not found

Notes:

(1) Based on total organic carbon concentration of 10,000 mg/kg (1%).
(2) South Division EPA Region 5 Ecological Screeening Level Sediment Screening Benchmark
(3) Value represents the PRG which is the sum of the parent material (RDX, HMX) and noted degradants

TABLE 3

LABORATORY ANALYTICAL CAPABILITY POLLING RESULTS

Parameter	Lab	Current	Modify	New
2,4,6-trinitrotoluene (TNT)	1	SW8330	NF	NF
2-amino-4,6-dinitrotoluene	1	SW8330	NF	NF
4-amino-2,6-dinitrotoluene	1	SW8330	NF	NF
2,6-Dinitrotoluene	1	SW8330	NF	NF
2,4-Dinitrotoluene	1	SW8330	NF	NF
2,6-Dinitrotoluene	1	SW8330	NF	NF
hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX)	1	SW8330	NF	NF
octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX)	1	SW8330	NF	NF
1,3,5-trinitrobenzene	1	SW8330	NF	NF
2,4,6-trinitrotoluene (TNT)	2	SW8330	NF	NF
2-amino-4,6-dinitrotoluene	2	SW8330	NF	NF
4-amino-2,6-dinitrotoluene	2	SW8330	NF	NF
1,3,5-trinitrobenzene	2	SW8330	NF	NF
2,4-Dinitrotoluene	2	SW8330	NF	NF
2,6-Dinitrotoluene	2	SW8330	NF	NF
hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX)	2	SW8330	NF	NF
octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX)	2	SW8330	NF	NF
formaldehyde	2	NA	NF	x
methanol	2	NA	NF	x
1,3,5-TRINITROBENZENE	3	SW8330	NF	NF
1,3-DINITROBENZENE	3	SW8330	NF	NF
2,2',4,4'-TETRANITRO-6,6'-AZOXYTOLUENE	3	SW8330M	NF	NF
2,2',6,6'-TETRANITRO-4,4'-AZOXYTOLUENE	3	SW8330M	NF	NF
2,4,6-TRINITROTOLUENE	3	SW8330	NF	NF
2,4-DIAMINO-6-NITROTOLUENE	3	SW8330	NF	NF
2,4-DINITROTOLUENE	3	SW8330	NF	NF
2,6-DIAMINO-4-NITROTOLUENE	3	SW8330	NF	NF
2,6-DINITROTOLUENE	3	SW8330	NF	NF
2-AMINO-4,6-DINITROTOLUENE	3	SW8330	NF	NF
4-AMINO-2,6-DINITROTOLUENE	3	SW8330	NF	NF
4-NITROTOLUENE	3	SW8330	NF	NF
DNX	3	SW8330	NF	NF
HMX	3	SW8330	NF	NF
MNX	3	SW8330	NF	NF
RDX	3	SW8330	NF	NF
TNX	3	SW8330	NF	NF

1 = Paragon
2 = Mitkem
3 = Laucks Laboratories
NA = Not applicable
NF = No feedback was received from the laboratory.
SW8330 = SW-846 Method 8330 for Nitramines and Nitroaromatics
SW8330M = Modified SW-846 Method 8330 for Nitramines and Nitroaromatics

Current: A method exists for quantifying the analyte at desired concentrations and the method is identified.
Modify: It is likely an existing method could be modified to quantify the anlayte at desired concentrations.
New: The laboratory believes a new methd would be required to quantify the analyte at desired concentrations.

TABLE 4

TYPICAL ABSORBANCE MAXIMA FOR SELECT CHEMICAL FUNCTIONAL GROUPS IN AQUEOUS SOLUTION

Name	Chromophore	Maximum Absorbance Wavelength(s) [nm]	Molar extinction, e	Source
acetylide	-C=C	175-180	6,000	1,2
Aldehyde	-CHO	210	1,500	1,2
amine	$-NH_2$	195	2,800	1,2
azo	-N=N-	285-400	3-25	1,2
bromide	-Br	208	300	1,2
carboxyl	-COOH	200-210	50 - 70	1,2
disulphide	-S-S-	194	5,500	1
ester	-COOR	205	50	1
ether	-O-	185	1,000	1,2
ketone	>C=O	195, 270-285	1,000	1,2
nitrate	$-ONO_2$	270	12	1
nitrile	-C=N	160	-	1
nitrite	-ONO	220 - 230	1000-2000	1
nitro	$-NO_2$	210	strong	1
olefin	C=C	190	NS	2
conjugated olefin	$(C=C)_2$	210-230		2
conjugated olefin	$(C=C)_3$	260		2

1 Downloaded from: http://hplc.chem.shu.edu/NEW/HPLC_Book/Detectors/det_uvab.html, 2/14/07.

2 Peters et al., 1974

Molar Extinction coefficients are in units of L/(mole*cm)

nm = nanometers

- = Not available

L/mole*cm = Liters per mole centimeter

TABLE 5

DEGRADATION PRODUCTS AND PARENT COMPOUND FOR RDX, TNT, AND HMX

DEGRADATION PRODUCT	Abbr	CASRN	PARENT COMPOUND			STANDARD ANALTICAL			Analyze Recommendation?	Justification
			RDX	TNT	HMX	8330B	8260B	8270C/D		
1,1-Dimethyl-Hydrazine	--	57-14-7	X		X	--	--	--	No	Standard Analytical Method for this degradation product is not currently available
1,2-Dimethyl-Hydrazine	--	540-73-8	X			--	--	--	No	Standard Analytical Method for this degradation product is not currently available
1,3,5-Trinitrobenzene	TNB	99-35-4		X		Y	--	--	Yes	Use existing standard analytical method for this degradation product
1-Hydroxylamino-3,5-Dinitro-1,3,5-Triazine	--	--	X			--	--	--	No	Standard Analytical Method for this degradation product is not currently available
1-Hydroxylamino-3,5-Dinitroso-1,3,5-Nitro-1,3,5-Triazine	--	--	X			--	--	--	No	Standard Analytical Method for this degradation product is not currently available
1-Hydroxylamino-3-Nitroso-5-Nitro-1,3,5-Triazine	--	--	X			--	--	--	No	Standard Analytical Method for this degradation product is not currently available
2,2',4,4'-Tetranitro-6,6'-Azoxytoluene	--	--		X		Y	--	--	Yes	Use existing standard analytical method for this degradation product
2,2',4,6'-Tetranitro-4,6'Azoxytoluene	--	--		X		Y	--	--	Yes	Use existing standard analytical method for this degradation product
2,2',6,6'-Tetranitro-4,4'Azoxytoluene	--	--		X		Y	--	--	Yes	Use existing standard analytical method for this degradation product
2,4,6-Triaminotoluene	TAT	634-87-7 (HCl)		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available
2,4,6-Trinitrobenzaldehyde	--	606-34-8		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available
2,4,6-Trinitrobenzonitrile	--	--		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available
2,4,6-Trinitrobenzyl Alcohol	--	--		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available
2,4-Diamino-6-Nitrobenzoic Acid	--	--		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available
2,4-Diamino-6-Nitrobenzyl Alcohol	--	--		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available
2,4-Diamino-6-Nitrotoluene	2,4-DANT	6629-29-4		X		Y	--	--	Yes	Use existing standard analytical method for this degradation product
2,4-Diaminonitrotoluene	2,4-DAT	--		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available
2,4-Dinitrotoluene	2,4-DNT	121-14-2		X		Y	--	--	Yes	Use existing standard analytical method for this degradation product
2,6-Diamino-4-Nitrotoluene	--	--		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available
2,6-Diamino-6-Nitrotoluene	2,6-DANT			X		Y	--	--	Yes	Use existing standard analytical method for this degradation product
2,6-Diaminonitrotoluene	2,6-DAT	--		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available
2,6-Dinitrotoluene	2,6-DNT	606-20-2		X		Y	--	--	Yes	Use existing standard analytical method for this degradation product
2-Amino-4,6-Dinitrotoluene	2-ADNT	35572-78-2		X		Y	--	--	Yes	Use existing standard analytical method for this degradation product
2-Amino-4-Nitrotoluene	2A-4NT	99-55-8		X		--	--	Y	Yes	Available analytical methods: SW-846 1625, SW-846 8270D, and EPA 8091 (by GC-ECD). Toxicity is not significant enough to warrant inclusion in the monitoring program.
2-Amino-6-Nitrotoluene	2A-6NT	603-83-8		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available

TABLE 5

DEGRADATION PRODUCTS AND PARENT COMPOUND FOR RDX, TNT, AND HMX
PAGE 2 OF 3

DEGRADATION PRODUCT	Abbr	CASRN	PARENT COMPOUND			STANDARD ANALTICAL			Analyze Recommendation?	Justification
			RDX	TNT	HMX	8330B	8260B	8270C/D		
2-Hydroxylamino-4,6-Dinitrotoluene	2-HADNT	59283-76-0		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available
2-Hydroxylamino-4-Nitrotoluene	2HA-4NT	--		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available
2-Nitroso-4-Nitrotoluene	--	--		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available
4,2'-Dinitro-2,6'Azoxytoluene	--	--		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available
4,6-Dinitro-4,6-Diaza-Hexanal	--	--	X			--	--	--	No	Standard Analytical Method for this degradation product is not currently available
4,6-Dinitroanthranil	--	--		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available
4-Amino-2,6-Dinitrobenzyl Alcohol	--	--		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available
4-Amino-2,6-Dinitro-M-Cresol	--	--		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available
4-Amino-2,6-Dinitrotoluene	4-ADNT	19406-51-0		X		Y	--	--	Yes	Use existing standard analytical method for this degradation product
4-Amino-2-Nitrotoluene	4A-2NT	119-32-4		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available
4-Hydroxylamino-2,6-Dinitrotoluene	4-HADNT	59283-75-9		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available
4-Hydroxylamino-2-Nitrotoluene	4HA-2NT	--		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available
4-Nitro-2,4-Diaza-Butanal	4-NDAB	--	X		X	--	--	--	No	Standard Analytical Method for this degradation product is not currently available
4-Nitroso-2-Nitrotoluene	--	--		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available
5-Hydroxy-4-Nitro-2,4-Diaza-Pentanal	--	--	X			--	--	--	No	Standard Analytical Method for this degradation product is not currently available
5-Nitro-M-Phenylenediamine	--	5042-55-7		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available
Bis(Hydroxymethyl)Nitramine	--	--			X	--	--	--	No	Standard Analytical Method for this degradation product is not currently available
Dimethyl-Nitrosoamine	--	62-75-9	X			--	--	--	No	Standard Analytical Method for this degradation product is not currently available
Formaldehyde	--	50-00-0	X		X	--	--	--	No	Available analytical methods: SW-846 8315A; ASTM D6303; EPA 556; and EPA 556.1 Toxicity is not significant enough to warrant inclusion in the monitoring program.
Hexahydro-1,3,5-Dinitroso-1,3,5-Triazine	DNX	--	X			Y	--	--	Yes	Use existing standard analytical method for this degradation product
Hexahydro-1,3,5-Mononitroso-1,3,5-Triazine	MNX	--	X			Y	--	--	Yes	Use existing standard analytical method for this degradation product
Hexahydro-1,3,5-Trinitroso-1,3,5-Triazine	TNX	13980-04-6	X			Y	--	--	Yes	Use existing standard analytical method for this degradation product
Hydrazine	--	302-01-2	X		X	--	--	--	No	Standard Analytical Method for this degradation product is not currently available
Hydroxymethyl-Hydrazine	--	--	X			--	--	--	No	Standard Analytical Method for this degradation product is not currently available
Methanol	--	50-00-0	X		X	--	Y	--	No	Toxicity is not significant enough to warrant inclusion in the monitoring program.

TABLE 5

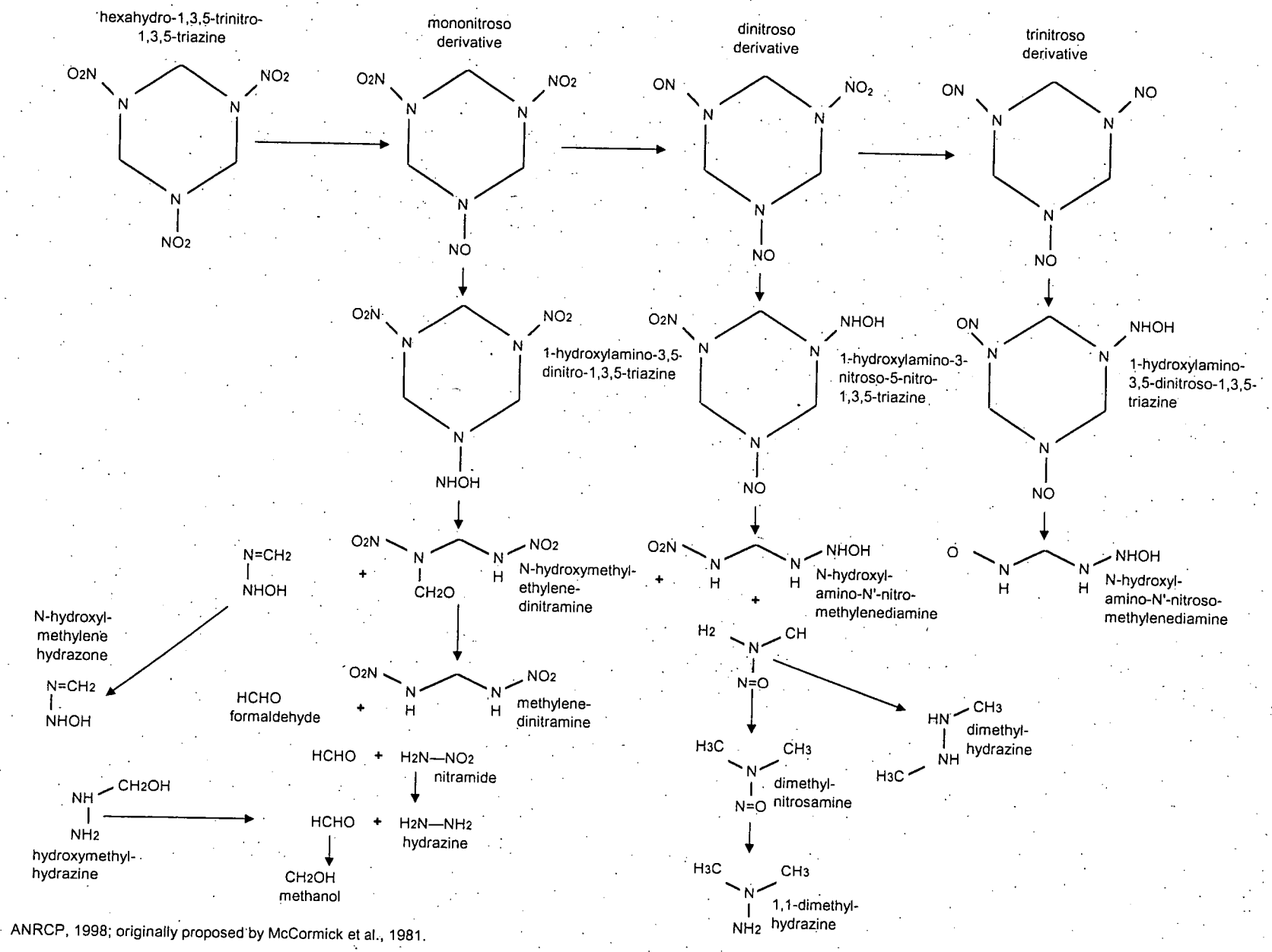
DEGRADATION PRODUCTS AND PARENT COMPOUND FOR RDX, TNT, AND HMX

DEGRADATION PRODUCT	Abbr	CASRN	PARENT COMPOUND			STANDARD ANALTICAL			Analyze Recommendation?	Justification
			RDX	TNT	HMX	8330B	8260B	8270C/D		
Methylene-Dinitramine	--	14168-44-6	X		X	--	--	--	No	Standard Analytical Method for this degradation product is not currently available
N-Hydroxyl-Amino-N'-Nitro-Methylenediamine	--	--	X			--	--	--	No	Standard Analytical Method for this degradation product is not currently available
N-Hydroxyl-Amino-N'-Nitroso-Methylenediamine	--	--	X			--	--	--	No	Standard Analytical Method for this degradation product is not currently available
N-Hydroxyl-Methylene Hydrazone	--	--	X			--	--	--	No	Standard Analytical Method for this degradation product is not currently available
N-Hydroxy-Methylethylene-Dinitramine	--	--	X		X	--	--	--	No	Standard Analytical Method for this degradation product is not currently available
Nitramide	--	7782-94-7	X		X	--	--	--	No	Standard Analytical Method for this degradation product is not currently available
Octahydro-1,3,5,7-Tetranitroso-1,3,5,7-Tetrazocine	--	--			X	Y	--	--	Yes	Use existing standard analytical method for this degradation product
Octahydro-1,3,5-Trinitroso-7-Nitro-1,3,5,7-Tetrazocine	--	--			X	--	--	--	No	Standard Analytical Method for this degradation product is not currently available
Octahydro-1,3-Dinitroso-5,7-Dinitro-1,3,5,7-Tetrazocine	--	--			X	--	--	--	No	Standard Analytical Method for this degradation product is not currently available
Octahydro-1,5-Dinitroso-3,7-Dinitro-1,3,5,7-Tetrazocine	dNs-HMX	--			X	--	--	--	No	Standard Analytical Method for this degradation product is not currently available
Octahydro-1-Nitroso-3,5,7-Trinitro-1,3,5,7-Tetrazocine	mNs-HMX	--			X	--	--	--	No	Standard Analytical Method for this degradation product is not currently available
Trinitrobenzoic Acid	TNBA	129-66-8		X		--	--	--	No	Standard Analytical Method for this degradation product is not currently available

Abbr - Abbreviation
CASRN - Chemical Abstract Services Registry Number.
TNT - 2,4,6-trinitrotoluene (CASRN: 118-96-7)
RDX - hexahydro-1,3,5-trinitro-1,3,5-triazine (CASRN: 121-82-4)
HMX - octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (CASRN: 2691-41-0)

-- Indicates intentionally left blank because method not applicable.
X - Indicates the parent compound for the degradation product.
Y - Indicates that the compound can be anayled by the listed method.

FIGURE 1
POTENTIAL RDX ANAEROBIC BIODEGRATION PATHWAYS



ANRCP, 1998; originally proposed by McCormick et al., 1981.

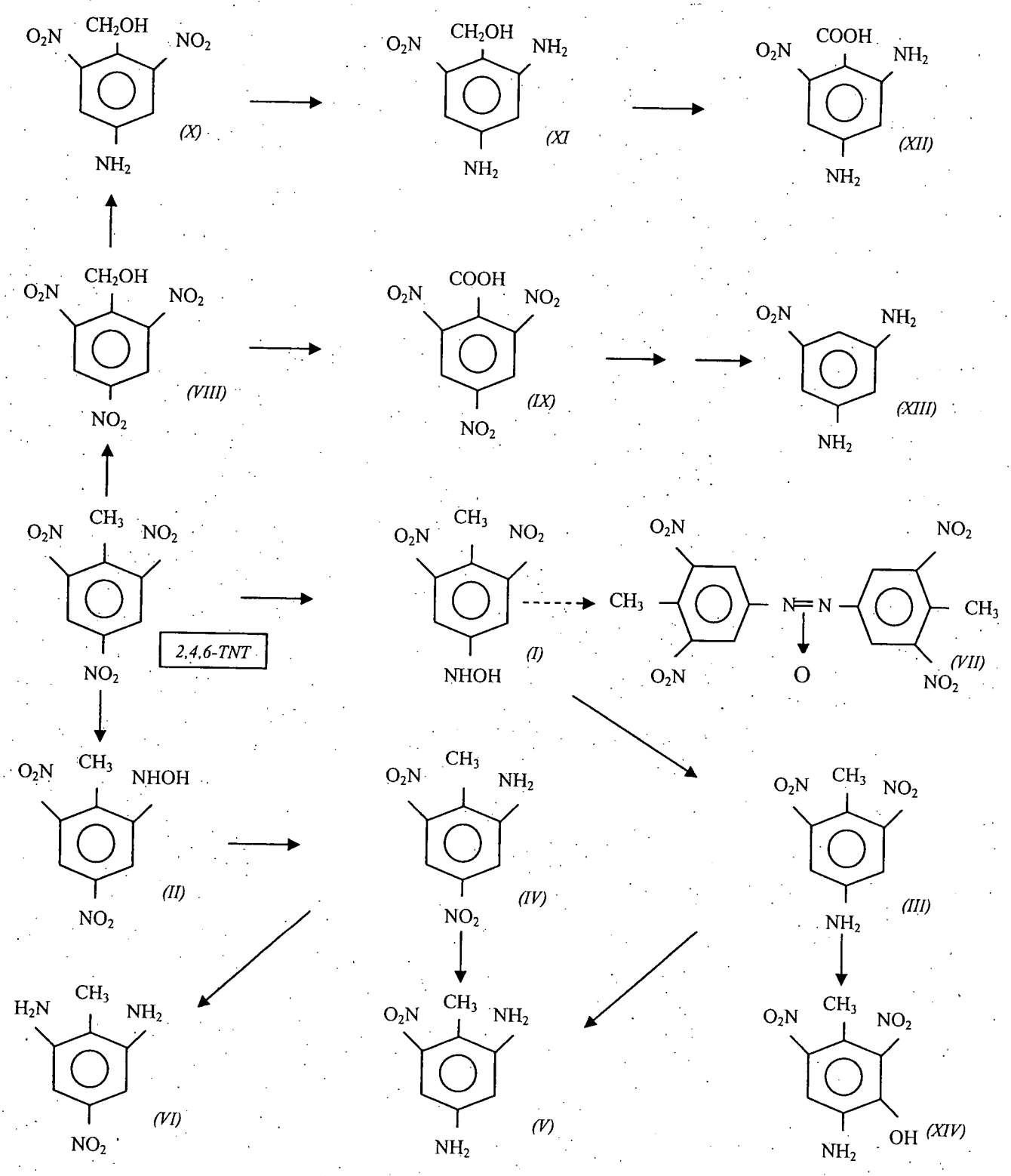


FIGURE 2

Possible biotransformation products of 2,4,6-TNT. (i) 4-hydroxylamino-2,6-dinitrotoluene; (ii) 2-hydroxylamino-4,6-dinitrotoluene; (iii) 4-amino-2,6-dinitrotoluene; (iv) 2-amino-4,6-dinitrotoluene; (v) 2,4-diamino-6-nitrotoluene; (vi) 2,6-diamino-4-nitrotoluene; (vii) 2,2',6,6'-tetranitro-4,4'azoxytoluene; (viii) 2,4,6-trinitrobenzylalcohol; (ix) trinitrobenzoic acid; (x) 4-amino-2,6-dinitrobenzylalcohol; (xi) 2,4-diamino-6-nitrobenzylalcohol; (xii) 2,4-diamino-6-nitrobenzoic acid; (xiii) 5-nitro-*m*-phenylenediamine; (xiv) 4-amino-2,6-dinitro-*m*-cresol. From ASTDR 1995a.

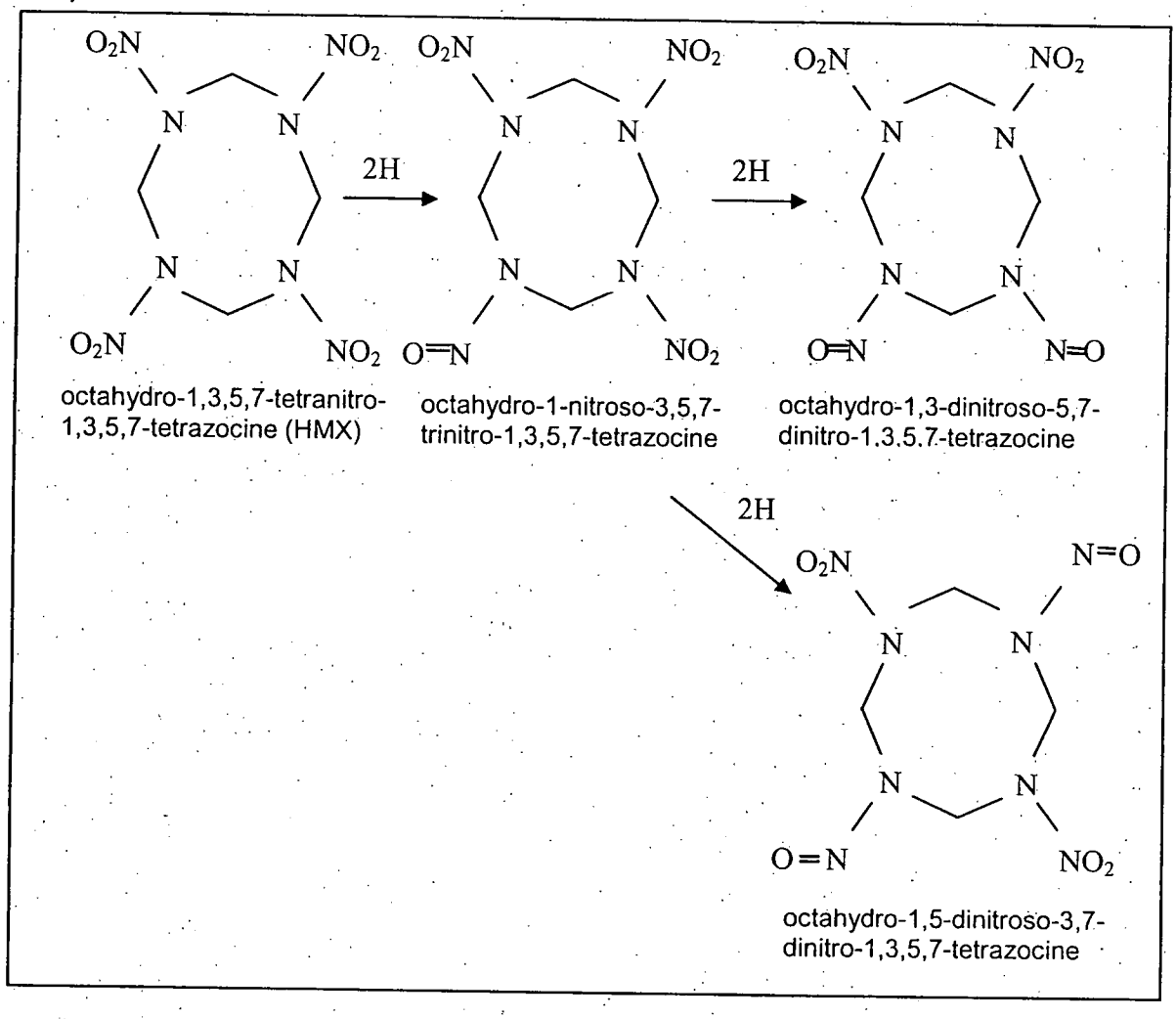


FIGURE 3

Proposed pathway for the formation of mono- and di-nitroso-derivatives of HMX from Kaplan, 1993 as cited in Card and Autenrieth, 1998.