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January 6, 2003

Christine Todd Whitman, Administrator
U.S. Environmental Protection Agency
P.O. Box 1473
Merrifield, VA 2216

Attn: Chemical Right-to-Know Program – Revised HPV Test Plan Submission – Mononitriles Category

Dear Administrator Whitman,

E. I. du Pont de Nemours & Company, Inc. submitted a proposed test plan along with the robust summary for the Mononitriles chemical category on November 12, 2002. We are resubmitting the cover letter, test plan and robust summary for this category with revisions to indicate that the cis- and trans- isomers of 2-Pentenenitrile are included in this submittal. Mononitriles included in this group are 2-Methyl-3-butenitrile (CAS# 16529-56-9), 2-Pentenenitrile (CAS# 13284-42-9), cis-2-Pentenenitrile (CAS# 25899-50-7), trans-2-Pentenenitrile (CAS# 26294-98-4), 3-Pentenenitrile (CAS # 4635-87-4) and 4-Pentenenitrile (CAS# 592-51-8). DuPont understands there will be a 120-day review period for the test plan and that all comments received by the EPA will be forwarded to us for consideration.

This submission includes one electronic copy in .pdf format and an electronic copy of the cover letter in Word format. Please replace the previously submitted copy of the cover letter, test plan and robust data summary with this revised version.

Please feel free to contact me with any questions or concerns you may have with regards to this revised submission at Edwin.L.Mongan-1@usa.dupont.com.

Sincerely,

Edwin L. Mongan, III
Manager, Environmental Stewardship
DuPont Safety, Health & Environment

Cc: Charles Auer – U.S. EPA
Office of Pollution Prevention & Toxics
U. S. Environmental Protection Agency
401 M Street, SW
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ROBUST SUMMARY FOR 5-CARBON MONONITRILE CATEGORY

Summary

Identification of a structure based category:

The mononitrile category is composed of linear straight and branched chain alkanes with a common functional group, nitrile, at one end of the parent alkane chain. This category is composed of individual isomers containing five carbon atoms that differ by the position of a carbon to carbon double bond relative to the nitrile group. Mononitriles included in this group are 2-methyl-3-butenitrile (2M3BN), 2-pentenenitrile (2-PN; including the cis and trans isomers), 3-pentenenitrile (3-PN; including the cis and trans isomers), and 4-pentenenitrile (4-PN). Structures of these mononitriles are presented below. Unless otherwise noted, data presented in this document for 2-PN and 3-PN will be for the mixture of the cis and trans isomers.

<u>Chemical Name</u>	<u>CAS Registry Number</u>	<u>Structure</u>
2-Methyl-3-butenitrile	16529-56-9	$\begin{array}{c} \text{CN} \\ \\ \text{CH}_3-\text{CH}-\text{CH}=\text{CH}_2 \end{array}$
2-Pentenenitrile	25899-50-7 (cis isomer) 26294-98-4 (trans isomer) 13284-42-9	$\text{CH}_3-\text{CH}_2-\text{CH}=\text{CH}-\text{CN}$
3-Pentenenitrile	4635-87-4	$\text{CH}_3-\text{CH}=\text{CH}-\text{CH}_2-\text{CN}$
4-Pentenenitrile	592-51-8	$\text{CH}_2=\text{CH}-\text{CH}_2-\text{CH}_2-\text{CN}$

The terminal nitrile group and limited chain length provide similar structure activity relationships with these materials. The mononitriles are synthesized in the production of adiponitrile, as a desired product (3-PN), by-product (2M3BN), process stream (2-PN), or impurity (4-PN). In the data summaries, information will be presented that indicate these liquid materials share similar physical chemical properties, environmental fate characteristics, ecotoxicity, and mammalian toxicity.

Scientific literature was searched and summarized (Table 1). Each study on category materials was evaluated for adequacy. Robust summaries were developed for each study addressing specific SIDS endpoints. Summaries were also developed for studies either considered not adequate but provided information of relevance for hazard identification and evaluation, or covered non-SIDS endpoints (Appendices A-D).

Table 1: Matrix of Available and Adequate Data for Mononitrile Category

	2-Methyl-3-butenitrile	2-Pentenenitrile	3-Pentenenitrile	4-Pentenenitrile
PHYSICAL/CHEMICAL CHARACTERISTICS				
Melting Point	N/A	N/A	N/A	N/A
Boiling Point	v	v	v	v
Vapor Pressure	v	v	v	v
Partition Coefficient (log Kow)	v	v	v	v
Water Solubility	v	v	v	v
ENVIRONMENTAL FATE				
Photodegradation	v	v	v	v
Stability in Water	v	v	v	v
Transport (Fugacity)	v	v	v	v
Biodegradation	v	v	v	v
ECOTOXICITY				
Acute Toxicity to Fish	v	v	v	v
Acute Toxicity to Invertebrates	v	v	v	v
Acute Toxicity to Aquatic Plants	-	v	-	v
MAMMALIAN TOXICITY				
Acute Toxicity	v	v	v	v
Repeated Dose Toxicity	v/-	v	v/-	v/-
Developmental Toxicity	-	v/-	-	-
Reproductive Toxicity	-	-	-	-
Genetic Toxicity Bacterial Gene Mutations	v/-	v	v/-	-
Genetic Toxicity Cellular Gene Mutations	-	v	-	-
Genetic Toxicity Chromosomal Aberrations	-	-	-	-
v = Data are available and considered adequate. v/- = Data available, but considered inadequate. - = No data available. N/A = Not applicable.				

Evaluation of Data Matrix Patterns:

The available data were broken out by discipline (physical chemical, environmental fate, ecotoxicology, and mammalian toxicology). These comparisons were conducted to determine if a pattern existed among the materials and to determine if additional testing needed to be conducted to complete the data set for the category.

All four mononitriles generally have equivalent physical chemical properties, as a result of structural similarity. Complete and adequate data (Table 2) correlate well with structure, and validate the category proposal.

Table 2: Physical and Chemical Characteristics*

	2-Methyl-3-butenenitrile	2-Pentenenitrile	3-Pentenenitrile	4-Pentenenitrile
Physical Appearance	Clear liquid, mild aromatic odor	Colorless liquid, pungent odor	Colorless to amber liquid	Liquid
Molecular Weight	81.12	81.12	81.12	81.12
Water Solubility	7850 mg/L @ 25°C (M) 6917 mg/L @ 22.5°C (E)	7930 mg/L @ 25°C (M) 7472 mg/L @ 22.5°C (E)	7930 mg/L @ 25°C (M) 7924 mg/L @ 22.5°C (E)	6794 mg/L @ 25°C (M)
Boiling Point	121-145°C	127°C	144-147°C	140°C
Vapor Pressure	11.1 mm Hg @ 25°C (M)	4.05 mm Hg @ 25°C (M)	4.05 mm Hg @ 25°C (M)	6.36 mm Hg @ 25°C (M)
Density/ Specific Gravity	0.8 @ 25°C	0.82 @ 20°C	0.83 @ 20°C	0.8239 @ 24°C
Partition Coefficient (Log Kow)	1.12 (M)	1.11 (M)	1.11 (M)	1.19 (M)
* Measured values are listed unless indicated as modeled (M) or estimated (E).				

Environmental fate data are essentially equivalent for the category members (Table 3). The data indicate that all 4 category members have a low potential for bioaccumulation. Biodegradation tests with 2M3BN, 2PN, and 3PN show that these test materials are not readily biodegradable, with biodegradation values of 8% after 21 days, 3% after 28 days, and 21% after 28 days, respectively. Fugacity modeling prediction for the mononitriles indicate these materials will act similarly in regard to partitioning to the environment. Modeled data show that all 4 test substances are essentially the same in terms of partitioning, with more material partitioning to the soil, and to a slightly lesser extent to water.

Table 3: Environmental Fate Data

	2-Methyl-3-butenitrile	2-Pentenenitrile	3-Pentenenitrile	4-Pentenenitrile
Bioaccumulation Potential*	Low BCF = 1.45	Low BCF = 1.44	Low BCF = 1.44	Low BCF = 1.65
Biodegradation	Not Readily Biodegradable	Not Readily Biodegradable	Not Readily Biodegradable	Biodegrades Fast*
Fugacity*	Air 1.9% Water 44.1% Soil 53.9% Sediments 0.09%	Air 10.8% Water 46.3% Soil 42.8% Sediments 0.01%	Air 0.5% Water 45.1% Soil 54.3% Sediments 0.1%	Air 1.5% Water 42.6% Soil 55.0% Sediments 0.09%
* Modeled data.				

Aquatic toxicity of the mononitrile category is generally low with actual or estimated acute endpoints of greater than 100 mg/L (Table 4). The estimated 4-PN acute toxicity data for fish, invertebrates, and algae are consistent with the test data for the other members of the class, and support the observed low concern for acute aquatic toxicity of members of the mononitrile class. No estimated or actual data exist on the aquatic toxicity of 3-PN or 2M3BN to algae, however, the algal test data for 2-PN and the estimated algal toxicity data for 4-PN are consistent, both with each other, and with the low observed or estimated toxicity of the other mononitriles to fish and invertebrates. Available test data for fish, invertebrates, and algae indicate that the acute toxicity of the mononitrile compounds is of low concern.

Table 4: Aquatic Toxicity

	2-Methyl-3-butenitrile	2-Pentenenitrile	3-Pentenenitrile	4-Pentenenitrile
Toxicity to Fish (96-hour LC ₅₀)	>100 mg/L (N)	316 mg/L (N)	>100 mg/L (N)	347 mg/L (E)
Toxicity to Invertebrates (48-hour EC ₅₀)	>100 mg/L (N)	114 mg/L (N)	>100 mg/L (N)	352 mg/L (E)
Toxicity to Algae (72-hour EC ₅₀)	No Data	263.5 mg/L (N)	No Data	210 mg/L (96-hour; E)
E = estimated value N = value based on nominal test concentrations				

The acute data that exists for these chemicals (Table 5) indicate that the chemicals produce similar toxicity profiles, with 2-PN and 3-PN being slightly more toxic than 2M3BN or 4-PN, and thus support a category approach. In mammalian species, 2M3BN and 4-PN exhibit slight toxicity via the oral and inhalation route, while 2-PN and 3-PN are moderately toxic. 2M3BN and 2-PN are moderately toxic via the dermal route, while no data is available for 3-PN or 4-PN. All 4 mononitriles are not skin irritants and are mild eye irritants, with the exception of 2-PN, which is a moderate eye irritant. Three of the 4 mononitriles are not skin sensitizers. No sensitization information is available for 2-PN; however, due to its structural similarity to the other members of the category, 2-PN is not expected to produce skin sensitization.

Table 5: Acute Mammalian Toxicity

	2-Methyl-3-butenitrile	2-Pentenenitrile	3-Pentenenitrile	4-Pentenenitrile
Oral ALD (rat)	1000 mg/kg	450 mg/kg	300 mg/kg	2250 mg/kg
Inhalation LC₅₀ (4-hour; rat)	3000 ppm	850 ppm	420 ppm	2550 ppm
Dermal LD₅₀	482 mg/kg	300 mg/kg*	No Data	No Data
Dermal Irritation	Not an irritant	Not an irritant	Not a primary irritant	Not an irritant
Eye Irritation	Mild	Moderate	Mild	Mild
Dermal Sensitization	Not a sensitizer	No Data	Not a sensitizer	Not a sensitizer
* Approximate Lethal Dose (ALD)				

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A summary of the available data regarding repeated dose, developmental, and reproductive toxicity is shown in Table 6. Ten 4-hour exposures at 55 ppm (3-PN), 550 ppm (4-PN), and 560 ppm (2M3BN) did not reveal a NOAEL for any of the test substances, due to observed clinical signs. However, there was no clinical or pathologic indication of accumulation in exposed rats, and no histological evidence of primary injury by any of the 3 test substances in any of the examined tissues was observed. A 4-week inhalation study with 2-PN revealed a NOAEL of < 3 ppm for male rats based on reduced body weights, 3 ppm for female rats based on microscopic nasal lesions and changes in sorbitol dehydrogenase activity, and 300 ppm for neurotoxicity in both male and female rats. In a 28-day oral study with 2-PN, no NOEL was reported. The lack of a NOEL was based on compound-related reductions in body weight and nutritional parameters, reductions in hindlimb grip strength (females only), and nasal lesions observed in male and female rats dosed with 10 mg/kg/day and above. Most parameters demonstrated at least partial reversal over a 2-month recovery phase; however, nasal histopathology did not demonstrate reversal.

Evaluation of developmental and reproductive toxicity for the mononitrile category cannot adequately be conducted with currently available data (Table 6). No studies have been conducted to examine the effects of any of these materials on developmental toxicity or male or female fertility. Histopathological evaluations of the gonads were conducted in some of the repeated dose studies, but were not sufficient to eliminate the possibility of an effect. Based on the similarity of results in acute and repeated dose studies for the mononitriles, it is anticipated that effects on fertility would be similar. As such it is proposed to evaluate the developmental and reproductive effects of 2-PN following OECD Guideline 422.

Table 6: Repeated Dose, Developmental, and Reproductive Toxicity

	2-Methyl-3-butenitrile	2-Pentenenitrile	3-Pentenenitrile	4-Pentenenitrile
Repeated Dose Toxicity (NOAEL)	<p>2-Week inhalation study:</p> <p>NOAEL not determined due to clinical signs at 560 ppm; no effects on body weight, mortality, or histopathology</p>	<p>4-Week inhalation study:</p> <p>NOAEL (male rats) < 3 ppm, based on body weight effects</p> <p>NOAEL (female rats) = 3 ppm, based on microscopic nasal lesions and changes in sorbitol dehydrogenase activity</p> <p>NOAEL (neurotoxicity, male and female rats) = 300 ppm</p> <p>28-Day oral study:</p> <p>NOEL not determined due to reduced body weight, nutritional parameters, hindlimb grip strength (females only), and evidence of nasal lesions at 10 mg/kg/day</p>	<p>2-Week inhalation study:</p> <p>NOAEL not determined due to clinical signs at 55 ppm; no effects on body weight, mortality, or histopathology</p>	<p>2-Week inhalation study:</p> <p>NOAEL not determined due to clinical signs at 550 ppm; no effects on body weight, mortality, or histopathology</p>
Developmental Toxicity	No Data	No Reliable Data	No Data	No Data
Reproductive Toxicity	No Data	No Data	No Data	No Data

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2-PN, 2M3BN, and 3-PN were tested in the Ames test for mutagenicity. 2-PN was non-mutagenic when tested with and without exogenous metabolic activation in all strains tested (TA97, TA98, TA100, TA1535, TA1537). 2M3BN was non-mutagenic with and without exogenous metabolic activation in all strains tested (TA98, TA100, TA1535, TA1537, and TA97), except TA97 (without activation), in which the results were considered weakly mutagenic or equivocal. 3-PN was non-mutagenic with or without activation in strains TA98, TA1535, and TA1537, but was weakly mutagenic or equivocal with and without activation in strains TA97 and TA100. Although data for a mouse lymphoma test with 2-PN is available, it does not satisfy the requirement for chromosomal aberration testing. In order for this test to be considered a clastogenicity test, colonies needed to be sized, and this was not performed; therefore, this test was considered a gene mutation test. No data regarding chromosomal aberrations is available for any of the mononitriles, therefore a chromosomal aberration study for 2-PN is recommended following OECD Guideline 473.

Table 7: Genetic Toxicity

	2-Methyl-3-butenitrile	2-Pentenenitrile	3-Pentenenitrile	4-Pentenenitrile
Mutagenic Potential (bacterial system)	Equivocal	Negative	Equivocal	No Data
Mutagenic Potential (tissue culture system)	No Data	Positive	No Data	No Data
Clastogenic Potential	No Data	No Data	No Data	No Data

Overall, the toxicological database for 2-pentenenitrile is nearly. The toxicological database for 2-methyl-3-butenitrile, 3-pentenenitrile, and 4-pentenenitrile are somewhat limited, but the information available suggests a level of toxicity comparable to 2-pentenenitrile. The 4 chemicals are similar in chemical structure, physical and chemical characteristics, environmental toxicity, aquatic toxicity, and acute toxicity, with 2-PN and 3-PN being slightly more toxic than 2M3BN and 4-PN. Because of these similarities, it is reasonable to conclude that the category members would behave similarly in the areas where data gaps are evident: biodegradation (4-PN), acute toxicity to invertebrates (4-PN), acute toxicity to aquatic plants (2M3BN, 3-PN), repeated dose (2M3BN, 3-PN, 4-PN), developmental toxicity (2M3BN, 2-PN, 3-PN, 4-PN), reproductive toxicity (2M3BN, 2-PN, 3-PN, 4-PN), genetic toxicity for bacterial mutagenicity (2M3BN, 3-PN, 4-PN), and chromosomal aberrations (2-PN, 2M3BN, 3-PN, 4-PN). To add further support to this category approach, where data gaps exist for all members of the category, a combined repeated dose study and developmental/reproductive toxicity screen (OECD Guideline 422), and an *in vitro* chromosome aberration assay (OECD Guideline 473) of 2-PN are recommended. Table 8 lists the proposed test plan for the mononitrile category.

Table 8: Mononitrile Proposed SIDS Test Plan

	2M3BN	2-PN	3-PN	4-PN
Combined Repeated Dose Study and Developmental/ Reproductive Toxicity Screen	–*	–	–*	–*
Genetic Toxicity Chromosomal Aberrations	–*	–	–*	–*
– = No data available. Testing recommended. * = Evaluation of the test substance will be considered based upon the results obtained from the study performed with 2-PN.				

Exposure Assessment

Mononitriles are synthesized in the production of adiponitrile (ADN). Mononitriles are manufactured at two facilities, the Victoria Site & Sabine River Works (SRW). 3-Pentenenitrile (3-PN; desired product) and 4-pentenenitrile (4-PN; impurity) are completely consumed as site-limited intermediates in the production of ADN. 2-Methyl-3-butenitrile (2M3BN) is a by-product and 99.75% is also consumed as a site limited intermediate in the production of ADN. The other 0.25% is sold to customers for use as a chemical intermediate in closed systems at industrial facilities. 2-Pentenenitrile (2-PN) is a stream from the ADN process where 83% is burned. 16.5% is sold to one customer for use as a chemical intermediate in a closed system at an industrial facility. 0.5% is sent to a toller that completely converts it to a new chemical.

DuPont facilities that produce mononitriles have effective safety, health & environmental practices and procedures in addition to engineering controls, environmental controls, and personal protective equipment to manage the risk of exposure. Both manufacturing facilities have from 250 to 2000 personnel (construction, contractor, and plant employees) working on site. The areas where the substances are manufactured have from 2 to 5 operators during normal operations and up to a total of 60 people during a shutdown or major construction activity. The toller and customers also have procedures, practices, and controls in place to manage the risk of exposure. DuPont assesses the ability of a potential toller to manage the risk of exposure prior to signing a contract and the contract specifies that any incidents must be reported to DuPont. DuPont also assesses the capability of a customer using the Product Stewardship Systems prior to selling a product. The Product Stewardship System works with customers around PPE (personal protective equipment), safety equipment (safety showers, eyewash stations, ventilation needs, etc.), storage concerns, disposal requirements, any MSDS questions, and getting an understanding of their application. No incidents have been reported to DuPont.

The potential for exposure is the greatest during the loading and unloading of the 2-PN and 2M3BN. Adequate safety equipment, such as safety showers, eyewash fountains, and washing facilities should be provided in the event of an occupational exposure.

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Individuals handling mononitriles should avoid contact with eyes, skin, and clothing, thoroughly wash any exposed area of the skin after handling, and avoid breathing any dust. Workers use butyl gloves and Tychem 9400 acid suits. They are not required to wear respirators during the routine operation of the plant. No sites or customers have reported any SHE incidents from the handling of 2-PN or 2M3BN.

Air monitoring has been conducted on 2-PN, 3-PN and 2M3BN. TWA samples are trapped using tertbutylcatechol treated charcoal tubes, desorbed with 5% acetone in carbon disulfide, and analyzed using gas chromatography. The accuracy of the overall analysis is reported to be 10% when the sampling pump is calibrated with a charcoal tube in line. LOGAN (lognormal analysis) is a computerized statistical method for characterizing occupational exposures to chemicals, noise, and other environmental hazards. LOGAN uses sequential collection of data and makes decisions on the minimum amount of data. It helps make cost-effective, accurate decisions that ensure a healthy workplace. LOGAN uses inferential statistics to estimate the true workplace conditions; in the same way that public polling estimates opinions by sampling a representative percentage of the public. LOGAN is designed to limit the risk of employee occupational overexposure to less than 5%.

No DuPont Acceptable Exposure Limit (AEL) is established for 2-pentenenitrile but it is strongly recommended that exposure be controlled using the AEL established for a related 2-PN product containing 80% cis-2-PN: 0.3 ppm, 8- and 12-hour TWA, skin. The DuPont Acceptable Exposure Limit for 3-pentenenitrile is 1 ppm 8- and 12-hour TWA, skin. No DuPont Acceptable Exposure Limit is established for 2-methyl-3-butenitrile or 4-pentenenitrile. None of the samples taken suggest the probability of exposure in excess of the recommended DuPont AEL's.

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EXPOSURE DATA

ADN PLANT

ADN Production Operators (No. of people = 88)				
<u>Chemical</u>	<u>No. of Results</u>	<u>Avg. of TWA (ppm)</u>	<u>Min. of Results (ppm)</u>	<u>Max. of Results (ppm)</u>
Methylbutenenitrile	134	0.0116	0.0096	0.1600
Pentenenitrile, 2-	134	0.0182	0.0096	0.7900
Pentenenitrile, 3-	134	0.0206	0.0096	0.2600

ADN I&E Maintenance (No. of people = 28)				
<u>Chemical</u>	<u>No. of Results</u>	<u>Avg. of TWA (ppm)</u>	<u>Min. of Results (ppm)</u>	<u>Max. of Results (ppm)</u>
Methylbutenenitrile	18	0.0099	0.0081	0.0100
Pentenenitrile, 2-	18	0.0099	0.0081	0.0100
Pentenenitrile, 3-	18	0.0105	0.0081	0.0200

ADN Maintenance Mechanics (No. of people = 39)				
<u>Chemical</u>	<u>No. of Results</u>	<u>Avg. of TWA (ppm)</u>	<u>Min. of Results (ppm)</u>	<u>Max. of Results (ppm)</u>
Methylbutenenitrile	91	0.0109	0.0081	0.0400
Pentenenitrile, 2-	91	0.0100	0.0081	0.0200
Pentenenitrile, 3-	91	0.0265	0.0081	0.7400

HMD PLANT

HMD Production Operators (No. of people 32)				
<u>Chemical</u>	<u>No. of Results</u>	<u>Avg. of TWA (ppm)</u>	<u>Min. of Results (ppm)</u>	<u>Max. of Results (ppm)</u>
Methylbutenenitrile	117	0.0128	0.0090	0.3500
Pentenenitrile, 2-	117	0.0099	0.0090	0.0100
Pentenenitrile, 3-	117	0.0108	0.0090	0.0500

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HMD I&E Maintenance (No. of people 12)				
<u>Chemical</u>	<u>No. of Results</u>	<u>Avg. of TWA (ppm)</u>	<u>Min. of Results (ppm)</u>	<u>Max. of Results (ppm)</u>
Methylbutenenitrile	10	0.0096	0.0082	0.0100
Pentenenitrile, 2-	10	0.0096	0.0082	0.0100
Pentenenitrile, 3-	10	0.0156	0.0082	0.0700

HMD Maintenance Mechanics (No. of people 20)				
<u>Chemical</u>	<u>No. of Results</u>	<u>Avg. of TWA (ppm)</u>	<u>Min. of Results (ppm)</u>	<u>Max. of Results (ppm)</u>
Methylbutenenitrile	22	0.0098	0.0094	0.0100
Pentenenitrile, 2-	22	0.0098	0.0094	0.0100
Pentenenitrile, 3-	22	0.0139	0.0094	0.0700

POWER HOUSE EAST

Power House Production Operators (No. of people 17)				
<u>Chemical</u>	<u>No. of Results</u>	<u>Avg. of TWA (ppm)</u>	<u>Min. of Results (ppm)</u>	<u>Max. of Results (ppm)</u>
Methylbutenenitrile	11	0.0100	0.0097	0.0100
Pentenenitrile, 2-	11	0.0100	0.0097	0.0100
Pentenenitrile, 3-	11	0.0100	0.0097	0.0100

OLA PACKAGING WAREHOUSE

Contractor Operators at the Packaging Warehouse and the Landfills packages waste solids and ships the solids to Landfill

Zachry/Sentinel Packaging Warehouse and SELF (No. of people 2)				
<u>Chemical</u>	<u>No. of Results</u>	<u>Avg. of TWA (ppm)</u>	<u>Min. of Results (ppm)</u>	<u>Max. of Results (ppm)</u>
Methylbutenenitrile	12	0.0093	0.0088	0.0100
Pentenenitrile, 2-	12	0.0093	0.0088	0.0100
Pentenenitrile, 3-	12	0.0093	0.0088	0.0100