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DATA EVALUATION REPORT

DIDECYL DIMETHYL AMMONIUM CHLORIDE
(Z-1)

STUDY TYPES: Product Identity and Composition (OPPTS 830.1550)
Description of Beginning Materials (OPPTS 830.1600)
Description of Formulation Process (OPPTS 830.1650)
Discussion of Formation of Impurities (OPPTS 830.1670)
Preliminary Analysis, Certified Limits (OPPTS 830.1700, 830.1750)
Enforcement Analytical Method (OPPTS 830.1800)
Physical and Chemical Characteristics (OPPTS 830.6302-830.7950)
MRID 44956001, 44956002, 44956003, 44956004, 44956005, 44956006

Prepared for
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Disclaimer

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Oak Ridge National Laboratory, managed by Lockheed Martin Energy Research Corp. for the U.S. Department of Energy under contract number DE-AC05-96OR22464.

SPONSOR: The Procter & Gamble Company, 5299 Spring Grove Avenue, Cincinnati, OH 45217

TESTING FACILITY: MRIDs 44956001 and 449560002: None given.

MRIDs 44956003, 44956004, 44956005, 44956006: ABC Laboratories, Inc., 7200 E. ABC Lane, Columbia, MO 65202

TITLE OF REPORT: MRID 44956001: Product Chemistry.

MRID 44956002: Storage Stability and Corrosion Characteristics.

MRID 44956003: Determination of Color, Physical State, Odor, pH, and Density (liquids) for SS0637.01.

MRID 44956004: Determination of Viscosity for SS0637.01.

MRID 44956005: Determination of the Oxidizing or Reducing Action and Chemical Incompatibility of SS0637.01.

MRID 44956006: Determination of the Flash Point for SS0637.01.

AUTHOR: MRIDs 44956001 and 44956002: M.D. Fritz and J.L. Dhonau.

MRIDs 44956003, 449560004, and 44956005: P. Sarff.

MRIDs 44956006: P. Sarff and L. Edgar.

REPORT ISSUED: MRIDs 44956001 and 44056002: October 21, 1999.

MRIDs 44956003 and 44956004: October 8, 1999.

MRIDs 44956005: October 7, 1999.

MRID 44956006: October 12, 1999.

EXECUTIVE SUMMARY: The product identity and composition, beginning materials and production process, formation of impurities, preliminary analysis, certified limits, enforcement analytical method, storage stability and corrosion characteristics, and physical and chemical characteristics for the end-use product Z-1 were addressed in MRIDs 44956001, 44956002, 44956003, 44956004, 44956005, and 4456006. Z-1 is used to kill odor-causing bacteria on hard-

INERT INGREDIENT INFORMATION IS NOT INCLUDED

to-launder products and is produced by either a batch or continuous process. No impurities are created during the formulation process, which is a simple blending of ingredients. CSFs were provided for a basic formulation and seven alternate formulations. All eight formulations contain the same amount of active ingredient and the same inerts, but vary on the source material for the active ingredient and on the amount of inerts. The basic formulation of Z-1 contains the active ingredient didecyl dimethyl ammonium chloride at a nominal concentration of 0.139% w/w, with certified lower-upper limits of 0.12-0.15%. The basic formulation of Z-1 also contains the following inerts: [redacted] Certified limits were generally within OPPTS suggested guidelines; an explanation was provided in the cases where the limits were exceeded. Preliminary analysis was not conducted because the product is not made by an integrated system. Details of the enforcement analytical method, which is based on titration, were provided.

Classification of studies:
Product Identity and Composition (OPPTS 830.1550)- **Acceptable**
Description of Beginning Materials (OPPTS 830.1600)- **Acceptable**
Description of Formulation Process (OPPTS 830.1650)-**Acceptable**
Discussion of Formation of Impurities (OPPTS 830.1670)- **Acceptable**
Preliminary Analysis (OPPTS 830.1700)- **Acceptable**
Certified Limits (OPPTS 830.1750)- **Acceptable**
Enforcement Analytical Method (OPPTS 830.1800)- **Acceptable**
Physical and Chemical Characteristics (OPPTS 830.6302-830.7950)-**Acceptable** for all characteristics except **Unacceptable** for storage stability and corrosion characteristics which are upgradeable upon receipt of data for a one-year trial.

COMPLIANCE: A Data Confidentiality statement was provided for each MRID. GLP compliance statements were provided for MRIDs 44956003, 44956004, 44956005, and 44956006. MRIDs 44956001 and 44956002 were not conducted in accordance with GLPs. Quality Assurance statements were provided for MRIDs 44956003, 44956004, 44956005, and 44956006. No quality assurance statement was provided for MRID 44956001 or 44956002.

A. PRODUCT IDENTITY AND COMPOSITION (OPPTS 830.1550)

Z-1 is an end-use product to kill odor-causing bacteria on hard-to-launder fabrics. It was submitted as a basic formulation and seven alternate formulations. The active ingredient is didecyl dimethyl ammonium chloride, which is 0.139% (w/w) of the product in the basic formulation (the source material is [redacted]. The

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basic formulation of Z-1 also contains the inert ingredients [redacted] The alternate formulations contain the same amount of active ingredient and the same inerts, but vary on the source material for the active ingredient and the amount of the inerts. The individual components of the perfumes were provided in MRID 44956001.

B. DESCRIPTION OF BEGINNING MATERIALS AND FORMULATION PROCESS (OPPTS 830.1600 AND OPPTS 830.1650)

Beginning materials and the production process are addressed in MRID 44956001. The quantities of beginning materials for a [redacted] The petitioner provided an MSDS for each of the beginning materials.

QUALITY CONTROL PROCEDURE INFORMATION IS NOT INCLUDED

MANUFACTURING PROCESS INFORMATION IS NOT INCLUDED

[redacted]

INERT INGREDIENT INFORMATION IS NOT INCLUDED

QUALITY CONTROL PROCEDURE INFORMATION IS NOT INCLUDED

[redacted]

C. DISCUSSION OF FORMATION OF IMPURITIES (OPPTS 830.1670)

No chemical reactions are expected and no impurities are created in the manufacture of Z-1, which is produced by a simple blending of the registered active ingredient with the inert ingredients.

MANUFACTURING PROCESS INFORMATION IS NOT INCLUDED

D. PRELIMINARY ANALYSIS (OPPTS 830.1700)

Not required because the end-use product is not produced by an integrated system [the active ingredient is an EPA-registered product [redacted]

E. CERTIFIED LIMITS (OPPTS 830.1750)

The Certified Limits for the basic formulation of Z-1 are: 0.12-0.15% (lower-upper, percent by weight) for the active ingredient, didecyl dimethyl ammonium chloride

[redacted]

The petitioner notes on page 4 of 9 of MRID 44956001 that Z-1 has not been produced in the petitioner's manufacturing facility and the certified limits are not optimized, but are based on the petitioner's knowledge of the raw materials and the capabilities of the manufacturing facilities, and may change in the future.

PRODUCT INGREDIENT SOURCE INFORMATION IS NOT INCLUDED

F. ENFORCEMENT ANALYTICAL METHOD (OPPTS 830.1800)

The enforcement analytical method is based on the dye-complexing property of cationic and anionic surfactants. A known amount of anionic surfactant is added to a sample of the cationic active ingredient in a graduated cylinder and the anionic and cationic surfactants complex, leaving an excess of the anionic surfactant. An indicator of cationic and anionic complexing dyes is then prepared in a water/methylene chloride system and added to the cylinder. The dye complex is soluble in the organic layer, giving it a red-pink color. The surfactant is then titrated with standardized benzethonium chloride, which destroys the dye-surfactant complex and the red-pink color. A color change to gray in the methylene chloride layer is the endpoint. A blue color in the organic layer indicates the solution is overtitrated. In tests of unadulterated product spiked with active product at 625-1875 ppm, recovery ranged from 95.0 to 97.9%, with an overall average of 96.8%. Example calculations were given in MRID 44956001.

G. PHYSICAL AND CHEMICAL CHARACTERISTICS (OPPTS 830.6302-830.7950)

The physical and chemical characteristics of the end-use product Z-1 were discussed in MRIDs 44956002, 44956003, 44956004, 44956005, and 4956006.

Color (830.6302): Value of N 8.75 and reflectance of 73.4% at 21.6° C (method reference given)

Physical State (830.6303): Liquid at 21.3° C (visual inspection)

Odor (830.6304): Flower-like and fruit or citrus-like at 20.5° C (by inspection)

Melting Point (830.7200): Not required for end-use products

Boiling Point (830.7220): Not required for end-use products

Density (830.7300): 0.9985 ± 0.0001 g/mL at 20° C with reference to water at 20° C (method reference given)

Solubility (830.7840): 0.76 ppm in water at 20° C (method reference given)

Vapor Pressure (830.7950): Not required for end-use products

Dissociation Constant (830.7370): Not required for end-use products

Octanol/Water Coefficient (830.7570): Not required for end-use products

pH (830.7000): 6.22 ± 0.142 at 20.1° C (1% w/w solution)

Stability (830.6313): For stability to normal and elevated temperature, see storage stability.

Oxidizing/reducing action (830.6314): No significant oxidizing/reducing action or chemical incompatibility occurred when mixed 1:1 (w/w) with potassium permanganate, zinc, monoammonium phosphate, turpentine, or water (method reference given)

Flammability (830.6315): Flash was not observed when flame was applied to vapors above the test substance up to the test substance's boiling point (~100°C) (method reference given)

Explodability (830.6316): Not applicable; the product contains no explosive components

Storage stability (830.6317): After 3 months storage in a high-density polyethylene container at 80° F, the concentration of the active product decreased from 1289 to 1207 ppm (6%) and the pH decreased from 3.77 to 3.72. After 6 months storage at 80° F, the concentration of active product decreased from 1289 to 1207 ppm (6%) and the pH was unchanged from the initial value. After 30 days storage in a high-density polyethylene container at 120° F, the concentration of active product decreased from 1289 ppm to 1253 ppm (3%) and the pH decreased from 3.77 to 3.71.

Viscosity (830.6318):1.3 cP at 30 rpm and at 60 rpm (method reference given)

Miscibility (830.6319): Not applicable; the product is not intended to be diluted with oil or other nonpolar solvents

Corrosion characteristics (830.6320): Upon microscopic examination after 30 days at 120° F, a high-density polyethylene container of Z-1 showed no visible differences from an unused container.

Dielectric breakdown voltage (830.6321): Not applicable; the product is not intended for use on or in the vicinity of electrical equipment

UV/Visible Absorption (830.7050): Not required for end-use products

MANUFACTURING PROCESS INFORMATION IS NOT INCLUDED

H. DISCUSSION

INERT INGREDIENT INFORMATION IS NOT INCLUDED

The product identity and composition, beginning materials and production process, formation of impurities, preliminary analysis, certified limits, and enforcement analytical method for Z-1 were addressed in MRID 44956001. The active ingredient is didecyl dimethyl ammonium chloride, and the inert ingredients are [redacted] and perfume. Z-1 was submitted in one basic and seven alternate formulations. The alternate formulations contain the same amount of active ingredient and the same inerts present in the basic formulation, but vary on the source material for the active ingredient and the amount of the inerts. The storage stability and corrosion characteristics were addressed in MRID 44956002, and the physical and chemical characteristics were addressed in MRIDs 44956003, 44956004, 44956005, and 4456006. Z-1 is produced by either a batch or continuous process. No impurities are created during the formulation process, which is a simple blending of ingredients. The certified limits for the active ingredient and most of the inerts are within OPPTS suggested guidelines; those for [redacted] and perfume are outside the range allowed by OPPTS 830.1750. The [redacted] The petitioner also stated that Z-1 has not been produced in their manufacturing facility, and that the proposed certified limits are based on the petitioner's knowledge of the raw materials and the manufacturing facility capabilities. Preliminary analysis was not performed and not needed because the product is not produced by an integrated system. Details of the enforcement analytical method, which is based on titration, were provided.

Classification of studies:

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Enforcement Analytical Method (OPPTS 830.1800)- **Acceptable**
Physical and Chemical Characteristics (OPPTS 830.6302-830.7950)- **Acceptable** for all characteristics except **Unacceptable** for storage stability and corrosion characteristics which are upgradeable upon receipt of data for a one-year trial.

I. STUDY DEFICIENCIES

The storage stability test was not conducted for the required period of one year and was not conducted according to the GLP requirement, and the corrosion characteristics test was not conducted for the recommended period of one year. A minor deficiency was that the purity of the active ingredient given on the CSF for alternate formulation 4 is [redacted] Also, all the CSFs identify one of the perfumes as [redacted] while page 78 of MRID 44956001 identifies it as [redacted]

INERT INGREDIENT INFORMATION IS NOT INCLUDED

PRODUCT INGREDIENT SOURCE INFORMATION IS NOT INCLUDE