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CONFIDENTIAL

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

JAN 25 1990

OFFICE OF
PESTICIDES AND TOXIC SUBSTANCES

MEMORANDUM

SUBJECT: Sostram Chemical Co. Response to the Simazine Reregistration Standard: Product Chemistry Data (MRID #41301901, DEB# 6237.)

FROM: R. B. Perfetti, Ph.D., Chemist
Reregistration Section
Dietary Exposure Branch
Health Effects Division (H7509C)

THRU: W. J. Boodee, Section Head
Reregistration Section
Dietary Exposure Branch
Health Effects Division (H7509C)

TO: Reto Engler, Ph.D., Chief
Science Analysis and Coordination Branch
Health Effects Division (H7509C)

and

J. Talarico, RM-74
Reregistration Branch
Special Review and Reregistration Division (H7508C)

Attached is the review of product chemistry data submitted by Sostram Chemical Co. in response to the simazine reregistration standard. This information was reviewed by Dynamac Corporation under supervision of Dietary Exposure Branch, HED.

The due date for this review was January 20, 1990.

This information has undergone secondary review in Dietary Exposure Branch and have been revised to reflect the Branch policies.

Please note that Attachment 2 to this review contains Confidential Appendices A, B, C, and , D. These are to be

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protected. Copies of these appendices wil be sent only to Toxicology Branch, Reregistration Branch (J. Talarico) and FOD (J. Burrell). All other copies will remain in this Branch.

Please note that revised Tables A and B are attached at the end of the review.

If you need additional input please advise.

Attachment 1: Review of Simazine Product Chemistry Data
Attachment 2: Confidential Appendices A,B,C and D

cc: With Attachments 1 and 2: R.B. Perfetti, R. Coberly (TOX), J. Burrell (FOD), Ethoprop Reregistration Standard File, Ethoprop Subject File, J.Talerico (RB, SR&RD)

cc: Without Attachments: P. Fenner-Crisp (HED), M. Hawkins (HED), F. Bishop (RD), Circulation (7), RF, R. Engler (SACB)

H7509C:DEB:X77484:CM#2:RM810:R.B.Perfetti:rp:1/24/89

DYNAMAC
CORPORATION

Final Report

SIMAZINE
Task 4: Registrant's Response to Product Chemistry Data Requirements

January 24, 1990

Contract No. 68-D8-0080

Submitted to:
Environmental Protection Agency
Arlington, VA 22202

Submitted by:
Dynamac Corporation
The Dynamac Building
11140 Rockville Pike
Rockville, MD 20852

SIMAZINE

REGISTRANT'S RESPONSE TO PRODUCT CHEMISTRY DATA REQUIREMENTS

Task - 4

BACKGROUND

In response to the Simazine Guidance Document, dated April 14, 1984, Sostram Chemical Company, a subsidiary of Oxon Italia S.P.A. of Italy, has submitted updated product chemistry data (1989; MRID 41301901) for the 95% technical (T) product (EPA Reg. No. 35915-10). These data and our conclusions are discussed below.

61-1. Product Identity and Disclosure of Ingredients

A Confidential Statement of Formula (CSF) has been submitted by the registrant (see Confidential Appendix A). These data do not satisfy the requirements of 40 CFR §158.155 (Guidelines Reference No. 61-1) regarding product composition for the Sostram 95% T (EPA Reg. No. 35915-10) because the CAS registry number and CA-approved chemical name was not provided for the active ingredient and impurities were incorrectly identified as inerts. Additional data are required for this topic.

61-2. Description of Beginning Materials and Manufacturing Process

The registrant has submitted the names and addresses of the suppliers, but not the specifications of the starting materials. The registrant has also submitted a description of the manufacturing process for the technical material (MRID 41301901). This information is reviewed in Confidential Appendix B. These data do not satisfy the requirements of 40 CFR §158.160 (Guideline Reference No. 61-2) regarding starting materials for the Sostram 95% T (EPA Reg. No. 35915-10) because the registrant did not describe the type of process (batch or continuous); furthermore, the registrant did not report specifications of starting materials, the pH and duration of the reaction, the identity of a solvent, quality control steps, or a description of the the process equipment. Additional data are required.

61-3. Discussion of Formation of Impurities

The registrant reported the name of an impurity formed during the synthesis of the technical product (MRID 41301901); this information is presented in Confidential Appendix C. This information does not satisfy the requirements of 40 CFR §158.167 (Guidelines Reference No. 61-3) regarding formation of impurities in the Sostram 95% T (EPA Reg. No. 35915-10) because the formation of the impurity was not adequately described and no

discussions were presented regarding carryover of impurities from the starting materials, solvent, or process intermediates. In addition, there was no discussion of post-production contamination or nitrosamine formation. Additional data are required.

62-1. Preliminary Analysis

The registrant has provided preliminary analyses of five batches each of the registered technical (MRID 41301901). The results of the preliminary analyses are discussed in Confidential Appendix D. These data do not satisfy the requirements of 40 CFR §158.170 (Guideline Reference No. 62-1) regarding preliminary analysis for the Sostram 95% T (EPA Reg. No. 35915-10) because no validation data or statements of precision and accuracy were provided for the methods used to obtain these data. Furthermore, no enforcement analytical method was submitted for [redacted] We note that no data were reported on the analysis of the product for nitrosamines. Additional data are required.

62-2. Certification of Limits

Certified limits reported in the CSF are presented in Confidential Appendix A. These data do not satisfy the requirements of 40 CFR §158.175 (Guidelines Reference No. 62-2) regarding certified limits for the Sostram 95% T (EPA Reg. No. 35915-10) because upper and lower limits were transposed between columns on the CSF. Furthermore, an explanation of how the certified limits were established for impurities was not provided. Additional data must be submitted.

62-3. Analytical Methods to Verify Certified Limits

[redacted]

No validation data or statements of precision and accuracy were reported. This description does not satisfy the requirements of 40 CFR §158.180 (Guideline Reference No. 62-3) regarding enforcement analytical methods for the Sostram 95% T (EPA Reg. No. 35915-10) because the registrant did not report validation data or a statement of precision and accuracy of the method.

The registrant has submitted analytical methods for the determination of other impurities in the technical product (MRID 41301901). The procedures are discussed in Confidential Appendix E. This information does not satisfy the requirements of 40 CFR §158.180 (Guideline Reference No. 62-3) regarding enforcement

analytical methods for the Sostram 95% T (EPA Reg. No. 35915-10) because the registrant did not submit a description and validation information of a method to determine an impurity of toxicological significance. Additional data are required.

PHYSICAL AND CHEMICAL CHARACTERISTICS

The physical and chemical characteristics for the technical product have been submitted by the registrant (MRID 41301901). These properties are presented in Table 1. Information submitted on color, physical state, odor, melting point, density, solubility, pH, and explodability are adequate. Data on the octanol/water partition coefficient are not adequate because the registrant did not specify whether the test material was pure active ingredient. No data were submitted for vapor pressure, stability, oxidizing or reducing action, storage stability, or corrosiveness. This constitutes a data gap.

Table 1. Physical and chemical properties of the simazine 95% T (EPA Reg. No. 35915-10). All data pertain to the technical grade of the active ingredient (TGAI; MRID 41301901).

Guidelines Reference No., 40 CFR §158.190; Name of Property		Description [Method]
63-2.	Color	white
63-3.	Physical state	homogeneous powder
63-4.	Odor	odorless
63-5.	Melting point	227-230 C
63-6.	Boiling point	Simazine is a solid at room temperature.
63-7.	Density, bulk density, or specific gravity	450-500 g/l
63-8.	Solubility	Solvent / Solubility / Temperature: water / 5 mg/l / 20 C; methanol / 400 g/kg / 20 C; chloroform / 900 g/kg / 20 C
63-9.	Vapor pressure	not submitted
63-10.	Dissociation constant	data not submitted
63-11.	Octanol/water partition coefficient	K_{ow} = 143 (log P = 2.15) [OECD Guideline]
63-12.	pH	7.5-9.5

(Continued.)

Table 1. (Continued.)

Guidelines Reference No., 40 CFR §158.190; Name of Property	Description [Method]
63-13. Stability	data not submitted
63-14. Oxidizing or reducing action	data not submitted
63-15. Flammability	not required for solids
63-16. Explodability	not explosive
63-17. Storage stability	no data submitted
63-18. Viscosity	simazine T is a solid at room temperature.
63-19. Miscibility	simazine T is a solid at room temperature.
63-20. Corrosiveness	not corrosive

TABLE A. GENERIC DATA REQUIREMENTS FOR THE SIMAZINE TECHNICAL GRADE OF THE ACTIVE INGREDIENT.[1]

Data Requirement	Test Substance[2]	Guideline Status	Must additional data be submitted under FIFRA Sec. 3(c)(2)(B)? [Yes]	[No]	Reference (MRID No.)
40 CFR §158.155-190 Product Chemistry					
Product Composition					
61-2. Beginning Materials & Production Process	TGAI	R	X[3]		41301901
61-3. Formation of Impurities	TGAI	R	X[4]		41301901
Analysis and Certification of Product Ingredients					
62-1. Preliminary Analysis	TGAI	CR	X[5]		41301901
Physical and Chemical Characteristics[6]					
63-2. Color	TGAI	R		X	41301901
63-3. Physical State	TGAI	R		X	41301901
63-4. Odor	TGAI	R		X	41301901
63-5. Melting Point	TGAI	R		X	41301901
63-6. Boiling Point	TGAI	N/A[7]		X	
63-7. Density, Bulk Density, or Specific Gravity	TGAI	R		X	41301901
63-8. Solubility	TGAI or PAI	R		X	41301901
63-9. Vapor pressure	TGAI or PAI	R	X		N/A
63-10. Dissociation Constant	TGAI or PAI	R	X		N/A
63-11. Octanol/Water Partition Coefficient	PAI	CR	X[8]		41301901
63-12. pH	TGAI	CR		X	41301901
63-13. Stability	TGAI	R	X		N/A
Other Requirements:					
64-1. Submittal of Samples	TGAI or PAI	CR		X[9]	N/A

TABLE A. (Continued).

1. Generic data requirements pertain to the TGAI of the Sostram Chemical Co. 95% T (EPA Reg. No. 35915-10). Additional data requirements are listed in the following Table B, "Generic Data Requirements for the Simazine 95% T (EPA Reg. No. 35915-10)", a registered technical product.

2. Test substance: MP = manufacturing-use product; PAI = purified active ingredient; TEP = typical end-use product; TGAI = technical grade of the active ingredient.

3. The following information must be provided: (i) a general characterization of the formulation or production process (e.g., batch or continuous); (ii) a description of a solvent used in the manufacturing process; (iii) a description of the equipment used; (iv) a description of the conditions (e.g., temperature, pressure, pH, humidity) that are controlled during each step of the process; and (v) a description of the procedures used to assure consistent composition of the substance produced (quality control methods); (vi) information concerning the composition of each starting material; and, (vii) a description of any purification procedures (including procedures to recover or recycle starting materials, intermediates or the substance produced).

4. A discussion regarding the origin of the following potential impurities must be provided: (i) each impurity associated with the active ingredient which was found to be present in any analysis of the product conducted by or for the registrant, and (ii) each impurity which the registrant has reason to believe may be present at a level equal to or greater than 0.1% (w/w) based on the composition of each starting material, intended and side reactions which may occur during production, the possible degradation of ingredients after production, post-production reactions between ingredients, possible contamination from packaging materials or production equipment, and process control, purification and quality control measures.

5. The registrant must provide complete and detailed descriptions of the methods used for sample analysis including statements of their precision and accuracy.

6. As required by 40 CFR §158.190 and more fully described in the Pesticide Assessment Guidelines, Subdivision D, Guidelines Reference Nos. 63-2 through 63-13, data must be submitted on physicochemical characteristics (color, physical state, odor, melting point, boiling point, specific gravity, solubility, vapor pressure, dissociation constant, octanol/water partition coefficient, pH, and stability). There are additional data requirements listed in Table B pertaining to physicochemical characteristics of those technical products which are also manufacturing use products.

7. Data on boiling point are not required since the technical product is a solid at room temperature.

8. The registrant must state whether the data reflect tests on the PAI.

9. If samples are required, the Agency will request them.

TABLE B. PRODUCT SPECIFIC DATA REQUIREMENTS FOR SIMAZINE MANUFACTURING-USE PRODUCTS.[1]

Data Requirement	Test Substance[2]	Guideline Status	Must additional data be submitted under FIFRA Sec. 3(c)(2)(B)? [Yes]	[No]	Reference (MRID No.)
40 CFR §158.155-190 Product Chemistry					
Product Composition					
61-1. Product Composition	MP	R	X[3]		41301901
61-2. Beginning Materials & Production/Formulation Process	MP	R	X[4]		41301901
61-3. Formation of Impurities	MP	R	X[5]		41301901
Analysis and Certification of Product Ingredients					
62-1. Preliminary Analysis	MP	CR	X[6]		41301901
62-2. Certified Limits	MP	R	X[7]		41301901
62-3. Enforcement Method	MP	R	X[8]		41301901
Physical and Chemical Characteristics[9]					
63-2. Color	MP	R		X	41301901
63-3. Physical State	MP	R		X	41301901
63-4. Odor	MP	R		X	41301901
63-7. Density, Bulk Density, or Specific Gravity	MP	R		X	41301901
63-12. pH	MP	CR		X	41301901
62-14. Oxidizing/Reducing Action	MP	CR	X[10]		N/A
62-15. Flammability	MP	CR		X[11]	N/A
63-16. Explodability	MP	R		X	41301901
63-17. Storage Stability	MP	R	X		N/A
63-18. Viscosity	MP	CR		X[12]	N/A
63-19. Miscibility	MP	CR		X[13]	N/A
63-20. Corrosion Characteristics	MP		X		41301901

(Continued, footnotes follow)

TABLE B. (Continued).

Data Requirement	Test Substance	Guideline Status	Must additional data be submitted under FIFRA Sec. 3(c)(2)(B)? [Yes] [No]	Reference (MRID No.)
Other Requirements:				
64-1. Submittal of Samples	MP	CR	X[14]	N/A

1. Data pertain to the Sostram 95% T (EPA Reg. No. 35915-10). Additional data requirements are listed in the preceding Table A, "Generic Data Requirements for the Simazine Technical Grade of the Active Ingredient", for the TGAI of the same product.

2. Test substance: MP = manufacturing-use product; PAI = purified active ingredient; TEP = typical end-use product; TGAI = technical grade of the active ingredient.

3. The registrant must report the CAS registry number and CA-approved chemical name of the active ingredient; furthermore, the registrant must amend the CSF so that all impurities are identified as such.

4. The following information must be provided: (i) a general characterization of the formulation or production process (e.g., batch or continuous); (ii) a description of a solvent used in the manufacturing process; (iii) a description of the equipment used; (iv) a description of the conditions (e.g., temperature, pressure, pH, humidity) that are controlled during each step of the process; and (v) a description of the procedures used to assure consistent composition of the substance produced (quality control methods); (vi) information concerning the composition of each starting material; and, (vii) a description of any purification procedures (including procedures to recover or recycle starting materials, intermediates or the substance produced).

5. A discussion regarding the origin of the following potential impurities must be provided: (i) each impurity associated with the active ingredient which was found to be present in any analysis of the product conducted by or for the registrant, and (ii) each impurity which the registrant has reason to believe may be present in the product at a level equal to or greater than 0.1% (w/w) based on the composition of each starting material, intended and side reactions which may occur in the production of the product, the possible degradation of ingredients in the product after production, post-production reactions between the ingredients in the product, possible contamination from packaging materials or production equipment, and process control, purification and quality control measures.

TABLE B. (Continued).

6. The registrant must provide complete and detailed descriptions of the methods used for sample analysis including statements of their precision and accuracy. In addition, all nitrosamines must be identified and quantified by methods sensitive to 1 ppm of N-nitroso contaminants in six samples of each manufacturing-use product; two samples of each must be analyzed shortly after production, two at 3 months after production, and two at 6 months after production. Upper limits must be proposed for all nitrosamines found.

7. The registrant must provide an explanation of how the certified limits reported on the Confidential Statement of Formula (CSF) were established (sample analysis using a validated analytical procedure, quantitative estimate based on the amounts of ingredients used, etc.) along with information on the accuracy and precision of any analytical procedures used. (Certified limits should be based on the sources and magnitude of variability in the manufacturing process and the stability of the ingredients following production.) In addition, the CSF must be amended so that upper and lower limits are no longer transposed between columns.

8. The registrant must provide an explanation of how the certified limits reported on the Confidential Statement of Formula (CSF) were established (sample analysis using a validated analytical procedure, quantitative estimate based on the amounts of ingredients used, etc.) along with information on the accuracy and precision of any analytical procedures used. (Certified limits should be based on the sources and magnitude of variability in the manufacturing process and the stability of the ingredients following production.) In addition, the CSF must be amended so that upper and lower limits are no longer transposed between columns.

9. As required in 40 CFR §158.190 and more fully described in the Pesticide Assessment Guidelines, Subdivision D, Guidelines Reference Nos. 63-2 through 63-20, data must be submitted on physicochemical characteristics of each manufacturing-use product (color, physical state, odor, specific gravity, pH, oxidizing or reducing action, flammability, explodability, storage stability, viscosity, miscibility, and corrosion characteristics). Additional data requirements regarding physicochemical properties of manufacturing-use products which contain only the technical grade of the active ingredient are listed in Table A, "Generic Data Requirements for the Simazine Technical Grade of the Active Ingredient."

10. Data are required on oxidizing/reducing potential if product contains an oxidizing or reducing agent.

11. Data are not required on flammability since the product does not contain combustible liquids.

12. Data on viscosity are required only if the product is a liquid.

13. Data on miscibility are required only if the product is an emulsifiable liquid and is to be diluted with petroleum solvents.

14. If samples are required, the Agency will request them.

Simazine product chemistry review

Page _____ is not included in this copy.

Pages 14 through 19 are not included in this copy.

The material not included contains the following type of information:

X Identity of product inert ingredients

X Identity of product impurities

X Description of the product manufacturing process

X Description of product quality control procedures

___ Identity of the source of product ingredients

___ Sales or other commercial/financial information

___ A draft product label

___ The product confidential statement of formula

___ Information about a pending registration action

___ FIFRA registration data

___ The document is a duplicate of page(s) _____

___ The document is not responsive to the request

The information not included is generally considered confidential by product registrants. If you have any questions, please contact the individual who prepared the response to your request.
