



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

FEB 20 1992

OFFICE OF
PESTICIDES AND TOXIC SUBSTANCES

MEMORANDUM

SUBJECT: Simazine 95% Technical (ID # 080807)
Oxon Italia S.P.A.: Response to the Simazine Guidance Document, dated 4/14/84: Product Chemistry.
(EPA Reg. No. 35915-10).
(MRID # 41676701; CBRS # 8184 and 8209;
DP BARCODE: D165841 and D165775).

From: Freshteh Toghrol, Ph.D., Chemist *F. Toghrol*
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Health Effects Division (H7509C)

THRU: William J. Hazel, Ph.D., Section Head *W. J. Hazel*
Reregistration Section II
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To: L. Rossi/ W. Waldrop PM Team 71 and 74
Reregistration Branch
Special Review and Reregistration Division (H7508W)

and

William L. Burnam, Acting Branch Chief
Science Analysis and Coordination Branch
Health Effects Division (H7509C)

Attached is a review of the Oxon Italia S.P.A. registered simazine 95% Product Chemistry data submitted in response to the Simazine Guidance Document, dated 4/14/84 and an Agency's memo (by R. Perfetti; CBRS #6237, dated 1/25/90). These data were reviewed by Dynamac Corporation under the supervision of the Chemistry Branch Reregistration Support, Health Effects Division (CBRS, HED).

This Dynamac review has undergone secondary review in CBRS and has been revised to reflect the Branch policies.

Please see our conclusions in the attached review regarding the adequacy of the information provided by the Registrant.

Revised Product Chemistry Data Tables are also included.

Attachment 1: Review of Simazine Product Chemistry Data 9 pages.
Attachment 2: Confidential Appendices A, B, C, D, and E of
Simazine Product Chemistry Data

cc With Attachment 1 and 2: Simazine S.F., Simazine
Reregistration Standard File , P. Deschamp, F. Toghrol, J.
Burrell/C. Furlow (PIB/FOD), and Dynamac.

cc (with Attachment 1): Circulate (7)

cc (without Attachments: Simazine R.F.

RDI: W. Hazel (2/119/92): E. Zager (2/19/92):
H7509C:CBII:RS:F.Toghrol:F.T.:RM:802:CM#2:(703)305-7887:9/10/91.

Final Report

**SIMAZINE (CBRS No. 8184 and 8209)
Shaughnessy No. 080807
Task 4: Registrant's Response to Product
Chemistry Data Requirements**

August 13, 1991

Contract No. 68-D8-0080

Submitted to:
Environmental Protection Agency
Arlington, VA 22202

Submitted by:
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SIMAZINE (CBRS NO. 8184 AND 8209)

SHAUGHNESSY NO. 080807

REGISTRANT'S RESPONSE TO PRODUCT CHEMISTRY DATA REQUIREMENTS

Task - 4

BACKGROUND

In response to the Simazine Guidance Document, dated 4/14/84 and an Agency Review (R. Perfetti; CBRS Memorandum No. 6237, dated 1/25/90), Oxon Italia S.P.A. has submitted a single volume of product chemistry data (CBRS Nos. 8184 and 8209; MRID 41676701) for the 95% simazine technical (T; EPA Reg. No. 35915-10). These data and our conclusions are discussed below.

PRODUCT IDENTITY AND COMPOSITION

61-1. Product Identity and Disclosure of Ingredients

A statement of composition has been submitted (1990; MRID 41676701) by the registrant for the product; the data are presented in Confidential Appendix A. These data do not satisfy the requirements of 40 CFR §158.155 (Guideline Reference No. 61-1) regarding product composition for the Oxon Italia 95% T (EPA Reg. No. 35915-10) because the purpose of the components other than simazine was not identified, and nominal concentrations were not submitted for the related impurities. Additional information is required for this topic.

61-2. Description of Starting Materials and Manufacturing Process

The registrant has submitted (1990; MRID 41676701) the names and addresses of the suppliers of the starting materials, and a detailed description of the manufacturing process for the product. A discussion of the current manufacturing process is given in Confidential Appendix B. These data do not satisfy the requirements of 40 CFR §158.160 and §158.162 (Guideline Reference No. 61-2) regarding starting materials and the manufacturing process for the 95% T (EPA Reg. No. 35915-10) because the registrant did not include the relative amounts and specifications of the starting materials. Additional data are required.

61-3. Discussion of Formation of Impurities

The registrant has submitted (1990; MRID 41676701) a discussion of formation of impurities including the possibility of the formation of nitrosamines during the production of the 95% T (EPA Reg. No. 35915-10). The discussion is presented in Confidential Appendix C, and satisfies the requirements of 40 CFR §158.167 (Guideline Reference No. 61-3) regarding discussion of formation of impurities in the 95% T. No additional data are required.

ANALYSIS AND CERTIFICATION OF PRODUCT INGREDIENTS

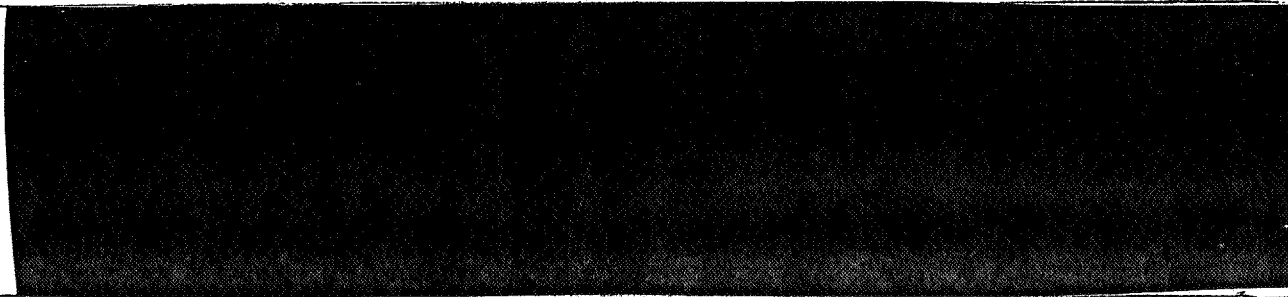
62-1. Preliminary Analysis

The registrant has submitted (1990; MRID 41676701) analyses of six batches of the 95% T (EPA Reg. No. 35915-10) for polar and non-polar nitrosamines. These data are discussed in Confidential Appendix D, and do not satisfy the requirements of 40 CFR §158.170 (Guideline Reference No. 62-1) regarding preliminary analysis of the 95% T because data were not submitted reflecting analysis for three components which are listed on the revised statement of composition. Although data previously reviewed by the Agency (R. Perfetti; CBRS Memorandum No. 6237, dated 1/25/90) included analysis for one of the compounds, new data are now required reflecting analysis for all components listed on the revised statement of composition. Additional data are required.

62-2. Certification of Limits

The registrant has submitted (1990; MRID 41676701) the certified limits for the active ingredient and impurities of the 95% T (EPA Reg. No. 35915-10). The data are presented in Confidential Appendix A and do not satisfy the requirements of 40 CFR §158.175 (Guideline Reference No. 62-2) regarding certification of limits for the 95% T because the limits for the active ingredient do not encompass the nominal concentration. The revised certified limits must be submitted on EPA Form 8570-4 (Rev. 2-85). Additional data are required.

62-3. Enforcement Analytical Methods



These data satisfy the requirements of 40 CFR §158.180 (Guideline Reference No. 62-3) regarding enforcement analytical methods for the 95% T (EPA Reg. No. 35915-10). No additional data are required.

PHYSICAL AND CHEMICAL CHARACTERISTICS

The full complement of physical and chemical characteristics for the 95% T has been submitted (1990; MRID 41676701) by the registrant; however, only data on vapor pressure, dissociation constant, octanol/water partition coefficient, stability, oxidizing/reducing action, storage stability, and corrosiveness remain outstanding from the previous submission (R. Perfetti; CBRS Memorandum No. 6237, dated 1/25/90). The required properties are presented in Table 1; the methods used for the determination of these characteristics were not included. The submitted data do not satisfy the requirements of 40 CFR §158.190 (Guideline Reference Nos. 63-2 through 63-20) pertaining to the physicochemical properties of the 95% T (EPA Reg. No. 35915-10) because raw data are required to support the submitted statements for stability, storage stability, and corrosiveness. In addition, the registrant must submit data depicting the stability of the TGA1 in the presence of sunlight, metals, and metal ions, and storage stability data reflecting at least one year's storage at warehouse conditions in the commercial container. Additional data are required.

Table 1. Physical and chemical properties of the simazine 95% T (EPA Reg. No. 35915-10) purified active ingredient (PAI), technical grade of the active ingredient (TGAI), and manufacturing-use product (MP). Data are from MRID 41676701.

Guidelines Reference No., 40 CFR §158.190; Name of Property	Description (Substrate)
63-9. Vapor pressure	0.812 uP at 20 C (TGAI)
63-10. Dissociation constant	pK = 1.72 at 20 C (TGAI)
63-11. Octanol/water partition coefficient	K _{ow} = 143 (log P = 2.15) (PAI)
63-13. Stability	stable in neutral and slightly acidic or basic conditions; at higher temperatures and in stronger acidic conditions simazine hydrolyzes to the hydroxy- derivative which is herbicidally inactive. (TGAI)
63-14. Oxidizing/ Reducing Action	does not contain an oxidizing or reducing agent (MP)
63-17. Storage Stability	stable at normal conditions; not to be stored above 50 C. (MP)
63-20. Corrosion Characteristics	not corrosive (MP)

TABLE A. GENERIC DATA REQUIREMENTS FOR THE SIMAZINE (OXON ITALIA S.P.A.) TECHNICAL GRADE OF THE ACTIVE INGREDIENT.

Data Requirement	Test Substance ²	Guideline Status	Must additional data be submitted under FIFRA Sec. 3(c) (2) (B)? [Yes] [No]	Reference (MRID No.)
<u>40 CFR §158.155-190 Product Chemistry</u>				
<u>Product Composition</u>				
61-2. Starting Materials and Manufacturing Process	TGAI	R	X ³	41676701
61-3. Formation of Impurities	TGAI	R	X	41676701
<u>Analysis and Certification of Product Ingredients</u>				
62-1. Preliminary Analysis	TGAI	CR	X ⁴	41676701
<u>Physical and Chemical Characteristics⁵</u>				
63-2. Color	TGAI	R	X	
63-3. Physical State	TGAI	R	X	
63-4. Odor	TGAI	R	X	
63-5. Melting Point	TGAI	R	X	
63-6. Boiling Point	TGAI	R	X ⁶	
63-7. Density, Bulk Density, or Specific Gravity	TGAI	R	X	
63-8. Solubility	TGAI or PAI	R	X	
63-9. Vapor pressure	TGAI or PAI	R	X	41676701
63-10. Dissociation Constant	TGAI or PAI	R	X	41676701
63-11. Octanol/Water Partition Coefficient	PAI	CR	X	41676701
63-12. pH	TGAI	CR	X	
63-13. Stability	TGAI	R	X ⁷	41676701
<u>Other Requirements:</u>				
64-1. Submittal of Samples	TGAI or PAI	CR	X ⁸	

1. Data requirements pertain to the Oxon Italia S.P.A. 95% T (EPA Reg. No. 35915-10). Additional data requirements are listed in the following Table B, "Generic Data Requirements for Simazine Manufacturing-Use Products", for registered technical products.

TABLE A. (Continued).

2. Test substance: MP = manufacturing-use product; PAI = purified active ingredient; TEP = typical end-use product; TGA1 = technical grade of the active ingredient.
3. Oxon Italia responded to data requirements for the 95% T; however, the relative amounts and specifications of the starting materials are required.
4. Oxon Italia has responded to data requirements for the 95% T; however, data were not submitted reflecting analysis for three components listed on the revised statement of composition. New data are required reflecting analysis for all components listed on the revised statement of composition.
5. 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.
6. Data are not required on this topic for the 95% T as the TGA1 is a solid at room temperature.
7. Oxon Italia has responded to data requirements for the 95% T; however, raw data supporting the submitted statements and data depicting the stability of the 95% T in the presence of sunlight, metals, and metal ions are required.
8. If samples are required the Agency will request them.

TABLE B. PRODUCT SPECIFIC DATA REQUIREMENTS FOR SIMAZINE (OXON ITALIA S.P.A.) MANUFACTURING-USE PRODUCTS.¹

Data Requirement	Test Substance ²	Guideline Status	Must additional data be submitted under FIRRA Sec. 3 (c) (2) (B)?		Reference (MRID No.)
			[Yes]	[No]	
<u>40 CFR §158.155-190 Product Chemistry</u>					
<u>Product Composition</u>					
61-1. Product Composition	MP	R	X ³		41676701
61-2. Storing Materials & Production/Formulation Process	MP	R	X ⁴		41676701
61-3. Formation of Impurities	MP	R		X	41676701
<u>Analysis and Certification of Product Ingredients</u>					
62-1. Preliminary Analysis	MP	CR	X ⁵		41676701
62-2. Certified Limits	MP	R	X ⁶		41676701
62-3. Enforcement Analytical Methods	MP	R		X	41676701
<u>Physical and Chemical Characteristics⁷</u>					
63-2. Color	MP	R		X	
63-3. Physical State	MP	R		X	
63-4. Odor	MP	R		X	
63-7. Density, Bulk Density, or Specific Gravity	MP	R		X	
63-12. pH	MP	CR		X	
62-14. Oxidizing/Reducing Action	MP	CR		X ⁸	41676701
62-15. Flammability	MP	CR		X ⁸	
63-16. Explodability	MP	R		X	
63-17. Storage Stability	MP	R	X ⁹		41676701
63-18. Viscosity	MP	CR		X ⁸	
63-19. Miscibility	MP	CR		X ⁸	
63-20. Corrosion Characteristics	MP	R	X ¹⁰		41676701

(Continued, footnotes follow)

TABLE B. (Continued).

Data Requirement	Test Substance ²	Guideline Status	Must additional data be submitted under FIFRA Sec. 3(c)(2)(B)?		Reference (MRID No.)
			[Yes]	[No]	

Other Requirements:64-1. Submittal of Samples MP CR X¹¹

1. Data requirements pertain to the Oxon Italia S.P.A. 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.

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

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3. Oxon Italia has responded to data requirements for the 95% T; however, the purpose of components other than simazine must be identified, and nominal concentrations must be submitted for related impurities.

4. Oxon Italia responded for the 95% T; however, the relative amounts and specifications of the starting materials are required.

5. Oxon Italia has responded to data requirements for the 95% T; however, data were not submitted reflecting analysis for three components listed on the revised statement of composition. New data are required reflecting analysis for all components listed on the revised statement of composition.

6. Oxon Italia has responded to data requirements for the 95% T; however, the proposed certified limits do not encompass the nominal concentration for the active ingredient. Revised certified limits must be submitted on EPA Form 8570-4 (Rev. 2-85).

7. 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, explosibility, 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."

TABLE B. (Continued).

8. Data are not required for the 95% T since the TGAI is a solid at room temperature.
9. Oxon Italia has responded to data requirements for the 95% T; however, data are required reflecting at least one year's storage at warehouse conditions in the commercial container.
10. Oxon Italia has responded to data requirements for the 95% T; however raw data must be submitted.
11. If samples are required the Agency will request them.

SIMAZINE (CBRS NOS. 8184 AND 8209)

PRODUCT CHEMISTRY

TASK 4

(Final Report)

CONFIDENTIAL APPENDICES

Appendix A:	1 Page(s)
Appendix B:	2 Page(s)
Appendix C:	1 Page(s)
Appendix D:	1 Page(s)
Appendix E:	1 Page(s)

Confidential Appendices to the Scientific Review of the Followup Report for the pesticide simazine by the Chemistry Branch II Reregistration Section [Confidential FIFRA Trade Secret/CBI].

SIMAZINE

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Page is not included in this copy.

Pages 14 through 19 are not included.

The material not included contains the following type of information:

- ☐ Identity of product inert ingredients.
- ☐ Identity of product impurities.
- ☐ Description of the product manufacturing process.
- ☐ Description of 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.

☒ CONFIDENTIAL appendix

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.
