Dockter
890.
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UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

OFFICE OF
PREVENTION, PESTICIDES AND
TOXIC SUBSTANCES

4/21/99

MEMORANDUM

SUBJECT: **Cacodylic Acid / Sodium Cacodylate.** PC Codes 012501 & 012502. List B Reregistration Case 2080. **Product Chemistry Chapter for the Reregistration Eligibility Decision.** DP Barcode D251099.

FROM: K. Dockter, Chemist
Reregistration Branch 2
Health Effects Division [7509C]
K. Dockter 4-21-99

THRU: Alan Nielsen, Branch Senior Scientist
Reregistration Branch 2
Health Effects Division [7509C]
Alan Nielsen 4/21/99

TO: Linda Werrell, PM 52
Special Review and Reregistration Division [7508C]

Attached is the Product Chemistry Chapter for the cacodylic acid [dimethylarsinic acid] / sodium cacodylate RED. The chapter was assembled by Dynamac Corporation under the supervision of RRB2, HED. The data assessment has undergone secondary and tertiary review and has been revised to reflect Agency policies. Four product chemistry data requirements remain outstanding.

Attachment: Reregistration Eligibility Decision: Product Chemistry Considerations

cc [with Attachment]: RF, List B File, SF. Dockter. Locke. Cropp-Kohlligian. Hart. Linda Werrell: SRRD.

[illegible] Smith. K. Dockter.

7509C:RRB2:CM2:Rm712N:57886:KD/kd.
CACODYLIC ACID.RED [890]

1

CACODYLIC ACID, AND SALT

REREGISTRATION ELIGIBILITY DECISION:

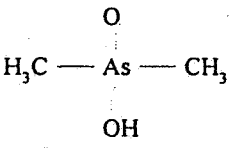
PRODUCT CHEMISTRY CONSIDERATIONS

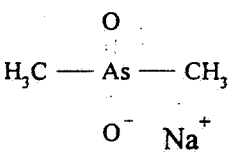
PC Codes 012501 and 012502; Case No. 2080

(DP Barcode D251099)

DESCRIPTION OF CHEMICAL

Cacodylic acid [dimethylarsinic acid] and its sodium salt, sodium cacodylate, are nonselective herbicides used in combination, primarily as a cotton defoliant.





Empirical Formula:	$C_2H_7AsO_2$	$C_2H_6AsNaO_2$
Molecular Weight:	137.99	159.99
CAS Registry No.:	75-60-5	124-65-2
PC Code:	012501	012502

NOTE: Chemical structures drawn by V. Hart, Technical Information Specialist, RRB2

IDENTIFICATION OF ACTIVE INGREDIENT

Cacodylic acid is a white crystalline solid with a melting point of 192-194 C, density of 1.10 g/mL, and octanol/water partition coefficient (P_{ow}) of <0.028 at 25 C. Cacodylic acid is soluble in water (102 g/100 mL at 25 C), and is very soluble in alcohol, less soluble in acetic acid, and practically insoluble in ether. Cacodylic acid is hygroscopic.

Sodium cacodylate is a white solid with a melting point of 77-79.5 C and density of 0.80 g/mL. Sodium cacodylate is soluble in methanol at 91.3 g/100 mL and is practically insoluble in hexane [illegible]

MANUFACTURING-USE PRODUCTS

A search of the Reference Files System (REFS) conducted 12/11/98 identified a single cacodylic acid/sodium cacodylate manufacturing-use product (MP) registered under PC Codes 012501 and

012502: the Luxembourg-Pamol, Inc. 5% cacodylic acid and 29% sodium cacodylate FI (EPA Reg. No. 42519-8). Because cacodylic acid is a list B chemical, only the cacodylic acid technical grade active ingredient [TGAI] and sodium cacodylate TGAI are subject to a reregistration eligibility decision.

REGULATORY BACKGROUND

The cacodylic acid and its sodium salt Phase 4 Review dated 3/6/91 by L. Cheng determined that additional data were required concerning starting materials and the production process, discussion of formation of impurities, preliminary analysis, certified limits, enforcement methods, stability, and solubility (OPPTS 830.1600, 1620, 1670, 1700, 1750, 1800, 6313, and 7840) for cacodylic acid, and that additional data were required for all guidelines except product identity (OPPTS 830.1550) for sodium cacodylate; product chemistry data submissions for remaining data requirements were determined to be acceptable for Phase 5 review. The Agency determined in the Phase 4 Review and in subsequent memoranda that a TGAI containing a mixture of cacodylic acid and sodium cacodylate would be acceptable to fulfill preliminary analysis data requirements, but that separate acid and salt test substances would be required to fulfill data requirements for physical/chemical properties.

The current status of the product chemistry data requirements for the cacodylic acid and sodium cacodylate TGAIs is presented in the attached data summary tables. Refer to these tables for a listing of the outstanding product chemistry data requirements.

CONCLUSIONS

Four product chemistry data requirements remain unfulfilled for the Luxembourg-Pamol cacodylic acid and sodium cacodylate TGAIs; additional data are required concerning starting materials, production processes, discussion of formation of impurities, and UV/visible absorption (OPPTS 830.1600, 1620, 1670, and 7050). Provided that the registrant submits the data required in the attached data summary tables for the cacodylic acid and sodium cacodylate TGAIs, and either certifies that the suppliers of beginning materials and the manufacturing processes have not changed since the last comprehensive product chemistry review or submits complete updated product chemistry data packages, HED has no objections to the reregistration of cacodylic acid and sodium cacodylate with respect to product chemistry data requirements.

AGENCY MEMORANDA CITED IN THIS DOCUMENT

CBRS No(s):	8865
DP Barcode(s):	D170691
Subject:	CCI Inc.: Response to the cacodylic Acid Phase IV Review: Product Chemistry Questions.
From:	R. Perfetti
To:	B. Crompton/B. Briscoe
Dated:	12/18/91
MRID(s):	None

CBRS No(s):	10279 and 10340
DP Barcode(s):	D180910 and D181087
Subject:	Cacodylic Acid and Sodium Cacodylate Reregistration: a List B Chemical (Chemical No.: 012501 and 012502; Case No. 2080). Luxembourg-Pamol: Response to the Cacodylic Acid and Sodium Cacodylate Phase 4 Review (dated 3/11/91) Product Chemistry (63 Series) Data Requirements.
From:	F. Toghrol
To:	B. Briscoe/B. Crompton
Dated:	12/23/92
MRID(s):	42397101 and 42403501

CBRS No(s):	10620, 10621, and 10634
DP Barcode(s):	D182857, D182869, and D182972
Subject:	Cacodylic Acid and Sodium Cacodylate Reregistration: a List B Chemical (Chemical No.: 012501 and 012502; Case No. 2080). Luxembourg-Pamol: Response to the Cacodylic Acid and Sodium Cacodylate Phase 4 Review (dated 3/11/91) Product Chemistry (63 Series) Data Requirements.
From:	F. Toghrol
To:	B. Briscoe/B. Crompton
Dated:	3/1/93
MRID(s):	40957801 and 42473801

CBRS No(s): 11236
DP Barcode(s): D187059
Subject: Cacodylic Acid and Sodium Cacodylate Reregistration: List B Chemical (Chemical No.: 012501 and 012502; Case No. 2080). Luxembourg-Pamol: Response to the Cacodylic Acid and Sodium Cacodylate Phase 4 Review (dated 3/11/91) Product Chemistry Data Requirements.
From: F. Toghrol
To: B. Briscoe/R. Kendall
Dated: 4/23/93
MRID(s): 42614501

CBRS No(s): 12828
DP Barcode(s): D196662
Subject: Cacodylic Acid and Sodium Cacodylate Reregistration: List B Chemical Nos. 012501 and 012502; Case No. 2080). Luxembourg-Pamol: Response to the Cacodylic Acid and Sodium Cacodylate Review (dated 4/20/93) Product Chemistry Data Requirements.
From: F. Toghrol
To: B. Briscoe/R. Kendall
Dated: 12/17/93
MRID(s): 42614501

PRODUCT CHEMISTRY CITATIONS

Bibliographic citations include only MRIDs containing data which fulfill data requirements.

References (cited):

40957801 Duescher, R. (1988) Determination of Stability: Laboratory Project ID HLA 6001-332. Unpublished study prepared by Hazleton Laboratories America, Inc. 18 p.

40957813 Bellet, E. (1988) Product Chemistry for 3.25 Cacodylate. Unpublished study prepared by Luxembourg-Pamol, Inc. 8 p.

41408202 Bellet, E. (1989) Cacodylate 3.25 Analytical Methods. Unpublished study prepared by Luxembourg-Pamol, Inc. 4 p.

42397101 Pesselman, R. (1992) Series 63 Product Chemistry Determinations of Cacodylic Acid (Melting Point, Solubility, Dissociation Constant, and Octanol/Water Partition Coefficient): Final Report: Lab Project Number: HWI 6366-107. Unpublished study prepared by Hazleton Wisconsin, Inc. 59 p.

42403501 Pesselman, R. (1992) Series 63 Product Chemistry Determinations of Sodium Cacodylate (Melting Point, Solubility, Dissociation Constant, and Stability): Final Report: Lab Project Number: HWI 6366-106. Unpublished study prepared by Hazleton Wisconsin, Inc. 54 p.

42473801 Bellet, E. (1992) Cacodylate 3.25: Physical and Chemical Characteristics. Unpublished study prepared by Chemical Consultants International, Inc. 5 p.

42614501 Shvo, Y. comp. (1992) Cacodylic Acid and Sodium Cacodylate: Preliminary Analysis and Certification of Limits: Cacodylate 3.25. Unpublished compilation prepared by Luxembourg Industries (Pamol), Ltd. 8 p.

92015001 Bellet, E. (1990) Luxembourg-Pamol Inc. U.S.A. Phase 3 Summary of MRID 40957813. Cacodylate 3.25: Product Identity and Composition. 11 p.

Case No. 2080
PC Code 012501

Case Name: Cacodylic Acid, and Salts
Registrant: Luxembourg-Pamol, Inc.
Product(s): Cacodylic acid TGAI

PRODUCT CHEMISTRY DATA SUMMARY

Guideline Number	Requirement	Are Data Requirements Fulfilled? [1]	MRID Number [2]
830.1550	Product identity and composition	N/A [3]	
830.1600	Description of materials used to produce the product	N [4]	92015001
830.1620	Description of production process	N [4]	92015001
830.1670	Discussion of formation of impurities	N	
830.1700	Preliminary analysis	Y	41608302, 42614501 [5]
830.1750	Certified limits	N/A [3]	
830.1800	Enforcement analytical method	N/A [3]	
830.6302	Color	Y	**40957813, 42473801**
830.6303	Physical state	Y	**40957813, 42473801**
830.6304	Odor	Y	**40957813, 42473801**
830.6313	Stability to normal and elevated temperatures, metals, and metal ions	N [6]	**40957801**
830.7000	pH	Y	**40957813, 42473801**
830.7050	UV/Visible absorption	N [7]	
830.7200	Melting point/melting range	Y	42397101 [8]
830.7220	Boiling point/boiling range	N/A [9]	
830.7300	Density/relative density/bulk density	Y	**40957813, 42473801**
830.7370	Dissociation constants in water	Y	42397101 [8]
830.7550	Partition coefficient (n-octanol/water), shake flask method	Y	42397101 [8]
830.7840	Water solubility: column elution method; shake flask method	Y	42397101 [8]
830.7950	Vapor pressure	N/A	

[1] Y = Yes; N = No; N/A = Not Applicable.

[2] **Bolded** references were reviewed under CBRS Nos. 10620, 10621, and 10634, D182857, D182869, and D182972, 3/1/93, F. Toghrol; underlined references were evaluated in the cacodylic acid and its sodium salt Phase 4 Review dated 3/6/91, L. Cheng for adequacy for Phase 5 review; and all other references were reviewed as noted.

[illegible]

Additional information concerning the following are required to upgrade the submission for Phase 5 review: (i) MSDSs for the starting materials used in the manufacture of the active ingredient; (ii) the concentration of the oxidizing reactant in the first step of the process; and (iii) temperatures for all the reaction and purification steps.

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[5] CBRS No. 11236, D187059, 4/23/93, F. Toghrol and CBRS No. 12828, D196662, 12/17/93, F. Toghrol.

[6] The test substance (acid or sodium salt) used for the stability study must be identified.

[7] The OPPTS Series 830, Product Properties Test Guidelines require data pertaining to UV/visible absorption for the PAI.

[8] CBRS Nos. 10279 and 10340, D180910 and D181087, 12/23/92, F. Toghrol.

[9] Data are not required because the TGAI is a solid at room temperature.

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Case No. 2080
PC Code 012502

Case Name: Cacodylic Acid, and Salts
Registrant: Luxembourg-Pamol, Inc.
Product(s): Sodium Cacodylate TGAI

PRODUCT CHEMISTRY DATA SUMMARY

Guideline Number	Requirement	Are Data Requirements Fulfilled? [1]	MRID Number [2]
830.1550	Product identity and composition	N/A [3]	
830.1600	Description of materials used to produce the product	N [4]	92015001
830.1620	Description of production process	N [4]	92015001
830.1670	Discussion of formation of impurities	N	
830.1700	Preliminary analysis	Y	41608302, 42614501 [5]
830.1750	Certified limits	N/A [3]	
830.1800	Enforcement analytical method	N/A [3]	
830.6302	Color	Y	**40957813, 42473801**
830.6303	Physical state	Y	**40957813, 42473801**
830.6304	Odor	Y	**40957813, 42473801**
830.6313	Stability to normal and elevated temperatures, metals, and metal ions	Y	42403501 [6]
830.7000	pH	Y	**42473801**
830.7050	UV/Visible absorption	N [7]	
830.7200	Melting point/melting range	Y	42403501 [6]
830.7220	Boiling point/boiling range	N/A [8]	
830.7300	Density/relative density/bulk density	Y	**40957813, 42473801**
830.7370	Dissociation constants in water	Y	42403501 [6]
830.7550	Partition coefficient (n-octanol/water), shake flask method	N/A [9]	
830.7840	Water solubility: column elution method; shake flask method	N/A [10]	
830.7950	Vapor pressure	N/A ?	

[1] Y = Yes; N = No; N/A = Not Applicable.

[2] **Bolded** references were reviewed under CBRS Nos. 10620, 10621, and 10634, D182857, D182869, and D182972, 3/1/93, F. Toghrol; underlined references were evaluated in the cacodylic acid and its sodium salt Phase 4 Review dated 3/6/91, L. Cheng for adequacy for Phase 5 review; and all other references were reviewed as noted.

[illegible] of the TGAI.

Additional information concerning the following are required to upgrade the submission for Phase 5 review: (i) MSDSs for the starting materials used in the manufacture of the active ingredient; (ii) the concentration of the oxidizing reactant in the first step of the process; and (iii) temperatures for all the reaction and purification steps.

[5] CBRS No. 11236, D187059, 4/23/93, F. Toghrol and CBRS No. 12828, D196662, 12/17/93, F. Toghrol.

[6] CBRS Nos. 10279 and 10340, D180910 and D181087, 12/23/92, F. Toghrol.

[7] The OPPTS Series 830, Product Properties Test Guidelines require data pertaining to UV/visible absorption for the PAI.

[8] Data are not required because the TGAI is a solid at room temperature.

[9] The Agency determined (CBRS No. 8865, D170691, 12/12/91, R. Perfetti) that data concerning this guideline are not required for sodium cacodylate.

[10] The Agency determined [Phase 4 Review, 3/6/91, L. Cheng] that data concerning this guideline are not required for sodium cacodylate.

"misquote"

82g salt/100g H_2O p17, EPA-540/1-75-021 Substitute Chml Prog, Initial Scientific Review of CA 12/75

to Do [illegible]