

US EPA ARCHIVE DOCUMENT

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REGISTRATION SUPPORT AND EMERGENCY RESPONSE BRANCH
REGISTRATION DIVISION (TS-767)

PRODUCT CHEMISTRY REVIEW ON NEW CHEMICALS

FROM: Bhushan Mandava, Ph.D., Chemist
Registration Support and
Emergency Response Branch

Bhushan Mandava
6/5/86

TO: Henry Jacoby (PM 21)
Registration Division

REQUESTOR: Stauffer Chemical Company = *MPID 150566*

REGISTRATION NO.: 476-859 ACCESSION NO. 259624


PESTICIDE CHEMICAL CODE: 039003 CAS REG. NO. 137-42-8

CHEMICAL NAME: Sodium Methylthiocarbamate

COMMON/TRADE NAME: Metham-sodium, Metam-sodium, VAPAM®

USE: Soil fumigant

PRODUCT CHEMISTRY: This product chemistry review addresses the response to a letter sent to Stauffer (dated 7/19/82) requesting further information in support of a registration application. The active ingredient (AI) in this product is identified, but a CAS based name is not given. A description of the manufacturing process is adequate. The purity of all the beginning materials is specified, but the source(s) and impurities, if any, of the beginning materials are not listed. The theoretical discussion of the formation of impurities covers all of the impurities noted from the analysis. The preliminary analyses of the technical grade active ingredient (TGAI) and the end-use product (EP) were completed. The impurities present in the EP are characterized. Analytical methods for enforcement are clearly explained, methods for quantification of all impurities noted and theorized are also included.

ADDITIONAL DATA NEEDED: 1) Source of beginning (starting) materials 

MANUFACTURING PROCESS INFORMATION IS NOT INCLUDED

MANUFACTURING PROCESS INFORMATION IS NOT INCLUDED

[REDACTED] material data safety sheets). 2) The dissociation constant of the TGAI and information on the melting point or decomposition of the TGAI. 3) A Confidential Statement of Formula (CSF) listing the active ingredient and its upper and lower certified limits, and upper certified limits for impurities present in concentrations of 0.1% or greater. The upper and lower certified limits of any intentionally added inert ingredients should also be included. 4) Submit samples of both the TGAI and the EP for validation of data.

RECOMMENDATION: Approve after submission of product specification sheets, dissociation constant, melting point or decomposition information, revised CSF, and samples.

Attachment

APPENDIX

EVALUATION OF THE PRODUCT CHEMISTRY DATA SUBMITTED

1. Product Identity- The applicant provided spectral data to support the claims for metam sodium. The evidence provided was IR (indicative of bands for N-H, C-S, and C-H stretching and bending vibration), NMR (a singlet methyl resonance), and UV [250 nm (λ_{max} 9200) and 282 nm (λ_{max} 11,400)]. The applicant should have provided a mass spectrum of the TGAI by field desorption mass spectrometry (which gives the molecular weight and other fragments corresponding to the structure) and ^{13}C NMR data for an unequivocal identification of the AI.

2. Manufacturing Process-

Although the byproducts arising from the beginning materials are fully accounted for, the impurities from the beginning materials are not discussed.

3. Discussion on Formation of Impurities- All the impurities in the TGAI were identified by MS (data given).

4. Analytical Methods for Verification of Certified Limits (Enforcement)- Metham in VAPAM[®] was determined by a titration method. Metham was converted to potassium methyl xanthate, which was titrated with iodine. Data presented on a sample of VAPAM[®] shows an average value of 33.19% metham (12 repetitive analyses) and a coefficient of variation of 0.3%. Water was analyzed by the Karl Fischer Method. Sodium content was determined by atomic absorption spectrometry.

MANUFACTURING PROCESS INFORMATION IS NOT INCLUDED

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PRODUCT SPECIFIC DATA FOR VA PAM[®]

- TECHNICAL
- MANUFACTURING USE PRODUCT
- END USE PRODUCT

EPA REGISTRATION NO. 476-859
 Table - §158.120 Product Chemistry Data Requirements

REGISTRATION GUIDELINE NO.	DATA REQUIREMENT	DATA RECEIVED FROM PM	COMMENTS BY RSERB CHEMIST
	<u>Product Identity:</u>		
61-1	Identity of Ingredients	} Yes	} See TGAT
61-2	Statement of Composition		
61-3	Discussion on Formation of Impurities		
	<u>Analysis and Certification of Product Ingredients:</u>		
62-1	Preliminary analysis	yes	Adequate
62-2	Certification of Limits	yes	Requires CGF
62-3	Analytical Methods for Enforcement of Limits	yes	Adequate
	<u>Physical and Chemical Characteristics</u>		
63-2	Color	yes	okay (colorless/yell)
63-3	Physical State	yes	solid/liquid
63-4	Odor	yes	ok (Rotten egg)
63-5	Melting Point	NO	N/A
63-6	Boiling Point	yes	ok (110°C)
63-7	Specific Gravity	yes	okay
63-8	Solubility	yes	ok at
63-9	Vapor Pressure	yes	okay
63-10	Dissociation Constant	NO	N/A
63-11	Octanol/Water Partition Coefficient	NO	N/A
63-12	pH	yes	okay (10.5)
63-13	Stability	NO	N/A
63-14	Oxidizing or Reducing Action	NO	N/A
63-15	Flammability	yes	okay (>110°)
63-16	Explosibility	yes	okay (not below)
63-17	Storage Stability	yes	okay
63-18	Viscosity	yes	okay
63-19	Miscibility	NO	N/A
63-20	Corrosion Characteristics	yes	okay
63-21	Dielectric Breakdown Voltage	NO	N/A

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PRODUCT CHEMISTRY REVIEW FOR NEW CHEMICALS

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PRODUCT SPECIFIC DATA FOR Meltham - Sodium

TECHNICAL

MANUFACTURING USE PRODUCT

END USE PRODUCT

EPA REGISTRATION NO. 476-859 - Only EP registration
 Table - §158.120 Product Chemistry Data Requirements

REGISTRATION GUIDELINE NO.	DATA REQUIREMENT	DATA RECEIVED FROM PM	COMMENTS BY RSERB CHEMIST
	<u>Product Identity:</u>		
61-1	Identity of Ingredients	Yes	Adequate
61-2	Statement of Composition	Yes	OKay
61-3	Discussion on Formation of Impurities	Yes	Need info for on beginning water
	<u>Analysis and Certification of Product Ingredients:</u>		
62-1	Preliminary analysis	Yes	Adequate
62-2	Certification of Limits	NO	N/R } Required only for EP.
62-3	Analytical Methods for Enforcement of Limits	NO	
	<u>Physical and Chemical Characteristics</u>		
63-2	Color	Yes	OKay
63-3	Physical State	Yes	OKay (solid)
63-4	Odor	Yes	
63-5	Melting Point	NO	Need melting pt. at composition point
63-6	Boiling Point	NO	N/A
63-7	Specific Gravity	NO	N/A
63-8	Solubility	Yes	OKay
63-9	Vapor Pressure	NO	N/R
63-10	Dissociation Constant	NO	Required
63-11	Octanol/Water Partition Coefficient	Yes	OKay
63-12	pH	NO	N/R (solid)
63-13	Stability	NO	N/R
63-14	Oxidizing or Reducing Action	}	}
63-15	Flammability		
63-16	Explosibility		
63-17	Storage Stability		
63-18	Viscosity		
63-19	Miscibility	}	}
63-20	Corrosion Characteristics		
63-21	Dielectric Breakdown Voltage		

Note to PM: Since the applicant is not seeking the 5 registration of TGA, the info. on phys. char. are adequate except the info. on melting/ decomposition point. Blumhan Handen

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PRODUCT CHEMISTRY INFORMATION FORM A

- 1. Product Name VAPAM®
- 2. EPA Reg. No. (if known) 476-859
- 3. Registrant Name Stauffer Chemical Company
- 4. Active Ingredient(s) Mefenamic Acid - Sodium

INFORMATION REQUESTED OF REGISTRANT	DATE	
	Req.	Rec.
1. Safety, Handling, & Storage Data	✓	
2. Analytical Method for Active Ingredient (A.I.)	✓	
3. Analytical Method for Specific Impurity	✓	
4. Analytical Grade Standard of A.I.	✓	
5. Analytical Standard of Specific Impurity*		
6. Technical Grade of A.I.*	✓	
7. MUPS Grade Material With A.I.*		
8. EUPS Grade Material With A.I.*	✓	
9. Melting Point		
10. Boiling Point		
11. Solubility of A.I.		
12. Spectral Data, IR	✓	
MS	✓	
NMR	✓	
13. Chromatographic Data, GLC		
HPLC		
14. Other	✓	

① Atomic absorption for sodium }
② Titration method }

*With Purity Statement

Blushman, Mandava
for PR 216

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PRODUCT CHEMISTRY INFORMATION FORM B

- 1. EPA Reg. No. 476-859
- 2. RD File No. 150
- 3. ACS Lab No. _____
- 4. Date Request Sent to ACS 6-6-86
- 5. Date Received by ACS _____
- 6. Date Assigned _____
- 7. Date of Follow-Up _____
- 8. Date Reported to RD _____

INFORMATION REQUESTED OF ACS

	DATE	
	Req.	Rec.
1. Validation of Active Ingredient Method	✓	
2. Validation of Method for Specific Impurity		
3. Validation of Melting Point		
4. Validation of Boiling Point		
5. Validation of Spectral Data, IR		
MS	✓	
NMR		
6. Validation of Chromatographic Data, GLC		
HPLC		
7. Other		

TGA and EP

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JUN 21

COMMUNICATION LOG ON REVERSE