

Shaughnessy No.: 068102

Date Out of EAB: JAN 23 1986

To: A. Castillo
Product Manager 31
Registration Division (TS-767)

From: Samuel M. Creeger, Chief 
Review Section #1
Exposure Assessment Branch
Hazard Evaluation Division (TS-769)

Attached, please find the EAB review of...

Reg./File #: 33677-R

Chemical Name: methylene bis(thiocyanate)

Type Product: microbiocide

Product Name: _____

Company Name: Tenneco Organics, LTD

Submission Purpose: Request for registration of technical product.

Date Received: 8/26/85

Action Code(s): 161

Date Completed: JAN 23 1986

EAB #(s) : 5896

days: 1.0

Deferrals to: _____ Ecological Effects Branch
_____ Residue Chemistry Branch
_____ Toxicology Branch

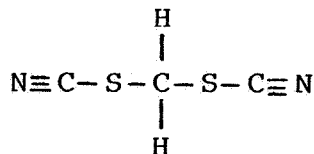
Monitoring study requested by EAB: ☐

Monitoring study voluntarily conducted by registrant: ☐

1. CHEMICAL:

Chemical name: methylene bis(thiocyanate)

Chemical structure:



Formulation: manufacturing-use product (99% pure)

Physical/Chemical properties:

appearance: white to crystalline solid
molecular weight: 130
melting point: 105-107°C
density: 2.0 g/ml
stability: stable to 100°C
reactivity: decomposes in alkaline solution
solubility (% w/w at 25°C):

acetone: 29
acetonitrile: 30
dimethylformamide: 44
dioxane: 24
ethylene glycol: 4
monoethyl ester: 17
methyl ethyl ketone: 20
water: 1

2. TEST MATERIAL: 99% technical (manufacturing-use product)

3. STUDY/ACTION TYPE:

Tenneco Inc. has submitted hydrolysis data in support of a request for registration of a 99% ai manufacturing-use product of methylene bis(thiocyanate).

4. STUDY IDENTIFICATION:

Macdonald, Ian A. and David A Howes (Huntingdon Research Centre Ltd., Huntingdon, Cambridgeshire, England). 1985. The determination of the hydrolysis of methylene bis thiocyanate as a function of pH - Report No. A & W 460/85626. (Unpublished study submitted by Tenneco, Inc; Accession no. 259005)

5. REVIEWED BY:

Debra Edwards, Ph.D.
Review Section 1/EAB/HED/OPP

Debra Edwards
JAN 23 1986

6. APPROVED BY:

Samuel M. Creeger, Chief
Supervisory Chemist
Review Section 1/EAB/HED/OPP

Sam M Creeger
JAN 23 1986

Methylene bis(thiocyanate), formaldehyde, and thiocyanate ion were measured at various intervals throughout the incubation period. Methylene bis(thiocyanate) was determined by HPLC using a Pye Unicam LC3 UV detector. Test solution peaks were compared to calibration curves developed for each pH at 5-50 ug/ml. For formaldehyde analysis, an aliquot of test solution was added to a solution of phenylhydrazine hydrochloride. Aqueous potassium ferricyanide was then added to oxidize the remaining phenylhydrazine to a magenta color. Optical density of the solution was measured at 517 nm and compared to calibration curves developed for pH 7 at 4-32 ug/ml and pH 9 at 15-90 ug/ml. Thiocyanate ion was determined using "Volhard's" titration. Excess silver nitrate and aqueous ammonium ferric sulfate (indicator) were added to the test solution, which was then titrated against ammonium thiocyanate to a brownish-red end point.

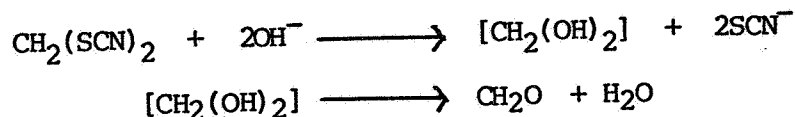
C. Reported Results:

The concentration of methylene bis(thiocyanate) at each sampling interval for each pH is given in Attachment 1. Methylene bis(thiocyanate) was stable at pH 5 and hydrolyzed at pH 7 and 9 with $t_{1/2}$ values of 21.2 hours and 133.5 minutes, respectively. Least squares linear regression was used to calculate $t_{1/2}$ values. Calculations for the pH 7 solution were made using the first three time points only, because the pH decreased throughout the sampling period (pH = 6.2 at 72 hours and 5.9 at 144 hours).

Concentrations of formaldehyde and thiocyanate ion were determined at 23 hours for pH 7 solutions and 265 and 445 minutes for pH 9 solutions. Data are presented in Attachments 2 and 3.

D. Study Authors' Conclusions:

The hydrolysis mechanism is described by the following equations:



"Methylene bis thiocyanate was found to be stable to hydrolysis at pH 5."

"Hydrolysis at pH 7 was found to occur with a half-life of 21.2 hours (average of two tests). The average rate constant was found to be $0.0327 \text{ hours}^{-1}$."

"Hydrolysis at pH 9 was found to occur with a half-life of 133.5 minutes (average of two tests). The average rate constant was $5.1894 \times 10^{-3} \text{ min}^{-1}$."

E. Reviewer's Discussion and Interpretation of Study Results:

The reviewer is in agreement with the study authors' conclusions. Although (i) a material balance was not provided for pH 7 or pH 9 solutions (reviewer calculated recoveries of 80% at pH 7 after 23 hours, and 59 and 68% at pH 9 after 265 and 445 minutes,

respectively); and (ii) the patterns of formation and decline of degradation products were not determined, the simple nature of the hydrolysis products formed will make repetition of this study unnecessary. (The fate of formaldehyde and thiocyanate ion are well known from the literature.) Therefore, for purposes of the registration request, the hydrolysis data requirement is satisfied.

11. COMPLETION OF ONE-LINER:

One-liner initiated (appended).

12. CBI APPENDIX:

No CBI appendix.

PAGES 5 THROUGH 7 HAVE BEEN REMOVED. THOSE PAGES CONSIST OF REGISTRANT-SUBMITTED DATA.