

Shaughnessy No.: 056502

Date Out of EFGWB:

MAR 31 1989

To: Larry Schnaubelt  
Product Manager PM #21  
Registration Division (H7505C)

From: Emil Regelman, Supervisory Chemist  
Environmental Chemistry Review Section #2  
Environmental Fate & Ground Water Branch/EFED (H7507C)

Thru: Henry Jacoby, Acting Chief  
Environmental Fate & Ground Water Branch/EFED (H7507C)

Attached, please find the EFGWB review of...

Reg./File # : 5481-197

Chemical Name: PCNB

Type Product : fungicide

Product Name : n.a.

Company Name : AMVAC Chemical Corporation

Purpose : Review hydrolysis study submitted in response to  
the 1987 Registration Standard.

Action Code: 660 EFGWB #(s): 90240

Date Received: 10/26/88 Total Reviewing Time: 2 days

Date Completed: 3/31/89

Monitoring Study Requested: \_\_\_\_\_

Monitoring Study Volunteered: \_\_\_\_\_

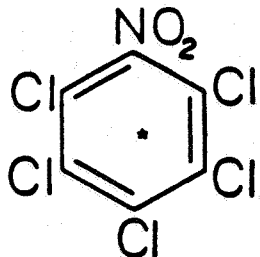
Deferrals to:  Ecological Effects Branch  
 Dietary Exposure Branch  
 Non-Dietary Exposure Branch  
 Toxicology Branch I  
 Toxicology Branch II

1. CHEMICAL:

chemical name: pentachloronitrobenzene

common name: PCNB

structure:



2. TEST MATERIAL:

<sup>14</sup>C-PCNB, 98.6% pure, specific activity: 46.4 mCi/mole

3. STUDY/ACTION TYPE:

Review a hydrolysis study submitted in response to the January 1987 PCNB Registration Standard.

4. STUDY IDENTIFICATION:

Bowman, Brian. "Determination of the Hydrolysis Rate of <sup>14</sup>C-PCNB." Performed by Analytical Bio-Chemistry Laboratories, Inc for AMVAC Chemical Corporation. Received by EPA on October 26, 1988. MRID #408653-01.

5. REVIEWED BY:

Dana Spatz  
Chemist, ECRS #2  
EFGWB/EFED/OPP

Date: MAR 31 1989

6. APPROVED BY:

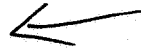
Emil Regelman  
Supervisory Chemist, ECRS #2  
EFGWB/EFED/OPP

Date: MAR 31 1989

7. CONCLUSIONS:

**Hydrolysis**

This study is acceptable and fulfills EPA Data Requirements for Registering Pesticides. PCNB is stable to hydrolysis in sterile, aqueous buffered solutions at pH's 5, 7, and 9 at 25°C in the dark. No significant degradation was observed at any pH during the conduct of the study. Quantification and characterization of residues was by TLC and GC-MS. The overall mean recovery for the study was 105 +8%.



8. RECOMMENDATIONS:

This study satisfies the hydrolysis data requirement (161-1) for PCNB as required by the 1987 Registration Standard.

9. BACKGROUND:

There are two registrants generating data separately in response to the registration standard: AMVAC and Uniroyal. This study was submitted by AMVAC.

PCNB is a non-systemic fungicide for soil and seed treatment for use on cotton, turf, cabbage, and peanuts. It is primarily applied as a spray or granular preparation to soil.

10. DISCUSSION OF INDIVIDUAL TESTS OR STUDIES:

See individual DER's.

11. COMPLETION OF ONE-LINER:

Updated one-liner is attached.

12. CBI APPENDIX:

Not applicable.

DATA EVALUATION RECORD

STUDY 1

161-1

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PCNB

BRANCH: ENVIRONMENTAL FATE & GROUND WATER

FORMULATION 00 - ACTIVE INGREDIENT

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Bowman, Brian. "Determination of the Hydrolysis Rate of <sup>14</sup>C-PCNB."  
Performed by Analytical Bio-Chemistry Laboratories, Inc for AMVAC Chemical  
Corporation. Received by EPA on October 26, 1988. MRID #408653-01.  
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DIRECT RVW TIME = 2

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REVIEWED BY: Dana S. Spatz  
TITLE: Chemist  
ORG: EFGWB/EFED/OPP  
TEL: 557-3463

SIGNATURE: 

MAR 31 1989

CONCLUSIONS:

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MATERIALS AND METHODS:

Preliminary Study:

A preliminary study was conducted to evaluate the proposed TLC method, evaluate sorption to test containers, evaluate the efficiency of extraction, and evaluate storage stability.

TLC method: acetonitrile/water/acetic acid (89:8:3)  
was chosen from a number of other systems  
for its ability to separate the possible  
degradates.

Sorption to test containers: Approximately 40% of the activity  
was lost due to sorption of PCNB to  
the culture tube.

Efficiency of extraction: 96.3% to 98.6% with hexane.

Storage stability: >6 weeks at pH 5 in either the refrigerator or a freezer.

Definitive Hydrolysis Study:

All buffer solutions (pH's 5, 7, and 9) and glassware were sterilized prior to addition of the test compound. The water employed in the study was taken from a Waters Milli-Q purification system. 1% acetonitrile was used as a co-solvent. Ten 5.0 ml aliquots of the test solutions (nominal 0.3 ug/ml) were placed in separate borosilicate glass vials and the vials were sealed. The test samples were placed in a temperature controlled (25  $\pm$ 1°C) environmental chamber in the dark.

The samples were assayed in duplicate on day 0, 7, 14, 22, and 30. Extraction was accomplished with hexane. The extracts were stored in a refrigerator prior to TLC, and a freezer afterwards.

Duplicate 100 ul aliquots were analyzed by LSC. Individual 100 ul aliquots of the extracts were spotted on Whatman C-18 rp-TLC plates and eluted as previously described.

The 30-day hexane extracts were analyzed on a Finnigan Model 5100 gas chromatograph/mass spectrometer.

**REPORTED RESULTS:**

**pH 5 <sup>14</sup>C-PCNB Hydrolysis Calculations**

Sample Day	Actual Time in Days	ug/ml in Extract	% Parent as Determined by RTLC	Parent Equivalents in ug/ml	Percent of Time 0	ln of % of Time 0
0	0	0.248	91.9%	0.228	100.0	4.61
7	6.79	0.243	95.7%	0.233	102.0	4.63
14	13.7	0.240	94.8%	0.228	99.8	4.60
22	21.9	0.242	95.0%	0.230	100.9	4.61
30	29.6	0.237	96.2%	0.228	100.0	4.61

$y = mx + b$

$t_{1/2} = \frac{-\ln 2}{k}$

$b = 4.61$

$k = |m| = -0.00014 \text{ day}^{-1}$

correlation coefficient = 0.0104

$t_{1/2} = 4705 \text{ days}$

**pH 7 (HEPES) <sup>14</sup>C-PCNB Hydrolysis Calculations**

Sample Day	Actual Time in Days	ug/ml in Extract	% Parent as Determined by RTLC	Parent Equivalents in ug/ml	Percent of Time 0	ln of % of Time 0
0	0	0.219	93.2%	0.204	100.0	4.61
7	6.79	0.157	92.0%	0.144	70.8	4.26
14	13.7	0.193	94.1%	0.182	89.0	4.49
22	21.9	0.187	93.8%	0.175	85.9	4.45
30	29.6	0.211	95.0%	0.200	98.2	4.59

$y = mx + b$

$t_{1/2} = \frac{-\ln 2}{k}$

$b = 4.44$

$k = |m| = +0.00235 \text{ day}^{-1}$

correlation coefficient = 0.157

$t_{1/2} = \text{no half-life calculated, slope is positive.}$

pH 7 (TRIS) <sup>14</sup>C-PCNB Hydrolysis Calculations

Sample Day	Actual Time in Days	ug/ml in Extract	% Parent as Determined by RLTC	Parent Equivalents in ug/ml	Percent of Time 0	In of % of Time 0
0	0	0.162	91.4%	0.148	100.0	4.61
7	6.79	0.158	92.3%	0.146	98.5	4.59
14	13.7	0.162	93.2%	0.151	102.0	4.62
22	21.9	0.160	93.0%	0.149	100.5	4.61
30	29.6	0.160	92.8%	0.148	100.3	4.61

$y = mx + b$

$t_{1/2} = \frac{-\ln 2}{k}$

$b = 4.60$

$k = |m| = +0.000327 \text{ day}^{-1}$

correlation coefficient = 0.0136

$t_{1/2}$  = no half-life calculated, slope is positive.

pH 9 <sup>14</sup>C-PCNB Hydrolysis Calculations

Sample Day	Actual Time in Days	ug/ml in Extract	% Parent as Determined by RLTC	Parent Equivalents in ug/ml	Percent of Time 0	In of % of Time 0
0	0	0.233	93.2%	0.217	100.0	4.61
7	6.79	0.240	94.4%	0.227	104.3	4.65
14	13.7	0.230	94.6%	0.218	100.2	4.61
22	21.9	0.228	95.1%	0.217	99.8	4.60
30	29.6	0.228	94.9%	0.216	99.6	4.60

$y = mx + b$

$t_{1/2} = \frac{-\ln 2}{k}$

$b = 4.62$

$k = |m| = -0.00070 \text{ day}^{-1}$

correlation coefficient = 0.0203

$t_{1/2} = 982 \text{ days}$

Mass Accountability of PCNB Hydrolysis Study - pH 5

Sample Day	ug/ml in Extracts		ug/ml in Post-Extracts		Total ug/ml Recovered	% Recovery
	Replicates	Mean	Replicates	Mean		
0	0.248 0.247	0.248	0.001 0.001	0.001	0.248	105.1%
7	0.243 0.242	0.243	0.001 0.001	0.001	0.243	103.0%
14	0.239 0.241	0.240	0.001 0.001	0.001	0.241	102.0%
22	0.240 0.244	0.242	0.001 0.001	0.001	0.243	102.8%
30	0.238 0.236	0.237	0.001 0.001	0.001	0.238	100.7%

% recovery based on measured test concentration of 0.236 ug/ml.

Mass Accountability of PCNB Hydrolysis Study - pH 7 (TRIS Buffer)

Sample Day	ug/ml in Extracts		ug/ml in Post-Extracts		Total ug/ml Recovered	% Recovery
	Replicates	Mean	Replicates	Mean		
0	0.162 0.162	0.162	0.001 0.001	0.001	0.163	106.4%
7	0.156 0.160	0.158	0.001 0.001	0.001	0.159	103.7%
14	0.163 0.160	0.162	0.001 0.001	0.001	0.162	106.1%
22	0.161 0.159	0.160	0.006 0.001	0.003	0.163	106.7%
30	0.156 0.163	0.160	0.001 0.001	0.001	0.161	104.9%

% recovery based on measured test concentration of 0.153 ug/ml.

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Mass Accountability of PCNB Hydrolysis Study - pH 7 (HEPES Buffer)

Sample Day	ug/ml in Extracts		ug/ml in Post-Extracts		Total ug/ml Recovered	% Recovery
	Replicates	Mean	Replicates	Mean		
0	0.220 0.217	0.219	0.000 0.001	0.000	0.219	127.3%
7	0.184 0.129	0.157	0.002 0.002	0.002	0.158	92.1%
14	0.179 0.207	0.193	0.002 0.002	0.002	0.195	113.4%
22	0.172 0.201	0.187	0.001 0.004	0.002	0.189	109.7%
30	0.196 0.226	0.211	0.003 0.001	0.002	0.213	123.8%

% recovery based on measured test concentration of 0.172 ug/ml.

Mass Accountability of PCNB Hydrolysis Study - pH 9

Sample Day	ug/ml in Extracts		ug/ml in Post-Extracts		Total ug/ml Recovered	% Recovery
	Replicates	Mean	Replicates	Mean		
0	0.235 0.231	0.233	0.001 0.001	0.001	0.234	101.2%
7	0.239 0.240	0.240	0.001 0.001	0.001	0.240	104.1%
14	0.234 0.225	0.230	0.001 0.001	0.001	0.230	99.7%
22	0.225 0.231	0.228	0.001 0.001	0.001	0.229	99.0%
30	0.223 0.233	0.228	0.001 0.001	0.001	0.229	99.1%

% recovery based on measured test concentration of 0.231 ug/ml.

VI

PCNB science review

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The material not included contains the following type of information:

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  - Identity of product impurities
  - Description of the product manufacturing process
  - 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
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**STUDY AUTHOR'S CONCLUSIONS:**

The results clearly indicate that PCNB is stable towards hydrolysis under study conditions of pH 5, 7, and 9.

**REVIEWER'S DISCUSSION:**

Although the sorption of PCNB to the walls of the sample container is significant (40%) and does reduce the amount available for hydrolysis, this study is acceptable because no significant degradation occurred at all, hence, the sorption to the glass would not affect the results of the study. In addition, one would not expect, from examining the chemical structure of PCNB, that hydrolysis would occur under the environmental conditions of the test.