DP Barcode:

Shaughnessy No.: 056502

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Thru: Henry Jacoby, Chief
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Attached, please find the EFGWB review of...

Reg./File # : 400-401, 5481-197

Chemical Name : Pentachloronitrobenzene

Type Product : Fungicide

Product Name : Terraclor

Company Name : Uniroyal and Amvac

Purpose : Response to 1987 Registration Standard.

Action Code : 660

Date Received : 8/28/90

EFGWB #(s): 90-0673, 0674, 0687-0690
0778, 0782, and 0819

Total Review Time: 14 days

Deferrals to:

__ Ecological Effects Branch

__ Dietary Exposure Branch

__ Non-Dietary Exposure Branch

__ Toxicology Branch I

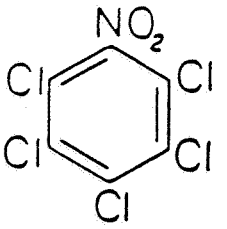
__ Toxicology Branch II

1. CHEMICAL:

chemical name: pentachloronitrobenzene

common name: PCNB

structure:



Formulations:

10-40% D, 75% WP, 2-30% G, 23.4-26.5% EC, 20% FlC, and 20-25% RTU-L.

Physical/Chemical properties:

Molecular formula: $C_6Cl_5NO_2$
Molecular weight: 295.3
Physical state: colorless needles
Density at 25°C: 1.718
Solubility at 25°C: 0.44 ppm in water, soluble in benzene and chloroform.
Vapor pressure at 25°C: 1.13×10^{-4} mm Hg
Melting point: 141-145°C

2. TEST MATERIAL:

See attached reviews of individual studies.

3. STUDY/ACTION TYPE:

Addendum to the PCNB Registration Standard.

4. STUDY IDENTIFICATION:

Bowman, B.R. 1988. Laboratory volatility from soil of PCNB. ABC Final Report No. 37090. Unpublished study performed by Analytical Bio-Chemistry Laboratories, Columbia, MO, and submitted by AMVAC Chemical Corporation, Los Angeles, CA. (41178001)

Bowman, B.R., and M. Fennessey. 1988. Determination of the hydrolysis rate of ^{14}C-PCNB. ABC Final Report No. 36005. Unpublished study performed by Analytical Bio-Chemistry Laboratories, Inc., Columbia, MO, and submitted by Uniroyal Chemical Company, Inc., Middlebury, CT. (40972601)

Cranor, W. 1989. Aerobic soil metabolism of ^{14}C-pentachloronitrobenzene. ABC Final Report No. 36824. Unpublished study performed by Analytical Bio-Chemistry Laboratories, Inc., Columbia, MO, and submitted by AMVAC Chemical Corporation, Los Angeles, CA. (41384501)

Daly, D., and W. Cranor. 1989. Aerobic soil metabolism of ^{14}C-pentachloronitrobenzene. ABC Final Report No. 35904. Unpublished study performed by Analytical Bio-Chemistry Laboratories, Inc., Columbia, MO, and submitted by Uniroyal Chemical Company, Inc., Middlebury, CT. (41203601)

Daly, D., and J. Schmidt. 1989. Anaerobic soil metabolism of ^{14}C-pentachloronitrobenzene. ABC Final Report No. 35905. Unpublished study performed by Analytical Bio-Chemistry Laboratories, Inc., Columbia, MO, and submitted by Uniroyal Chemical Company, Inc., Naugatuck, CT. (41203602)

Forbis, A.D. 1988. Uptake, depuration, and bioconcentration of ^{14}C-PCNB to bluegill sunfish (Lepomis macrochirus). Laboratory Project ID ABC #35965. Unpublished study performed by Analytical Bio-Chemistry Laboratories, Columbia, MO, and submitted by Uniroyal Chemical Company, Middlebury, CT. (40580202)

Forbis, A.D. 1990. Bioconcentration of ^{14}C-PCNB to channel catfish (Ictalurus punctatus) and bluegill (Lepomis macrochirus) under static uptake conditions. ABC Final Report No. 37033. Unpublished study performed by Analytical Bio-Chemistry Laboratories, Columbia, MO, and submitted by AMVAC Chemical Corporation, Los Angeles, CA. (41521001)

Halls, T.D.J. 1990. Confined accumulation on ^{14}C-PCNB of rotational crops treatment, sampling and combustion analysis. Uniroyal Project No. 8755. ABC Laboratories Final Report No. 35971. Unpublished study performed by Analytical Bio-chemistry Laboratories, Columbia, MO; and submitted by Uniroyal Chemical Company, Incorporated, Middlebury, CT. (41562905)

Irissarri, G. and M. Lengen. 1989. Field dissipation of pentachloronitrobenzene on a California turf site. Uniroyal Project No. 8785. Unpublished study performed by California Agricultural Research, Inc., Kerman, CA; North Coast Laboratories, Inc., Arcata, CA; and Uniroyal Chemical Co., Inc., Middlebury, CT; and submitted by Uniroyal Chemical Co., Inc., Middlebury, CT. (41210501)

Rice, F., B. Jacobson, and M.W. Winberry. 1989a. Terrestrial field dissipation for PCNB in broccoli. Uniroyal Project No. 8754B. Unpublished study performed by Pan Agricultural Laboratories, Madera, CA and Analytical Bio-Chemistry Laboratories, Inc., Columbia, MO; and submitted by Uniroyal Chemical Co., Inc., Middlebury, CT. (41216401)

Rice, F., B. Jacobson, and M.W. Winberry. 1989b. Terrestrial field dissipation for PCNB in peanuts. Uniroyal Project No. 8754A. Unpublished study performed by Southern Agricultural Research, Inc., Donalsonville, GA and Analytical Bio-Chemistry Laboratories, Inc., Columbia, MO; and submitted by Uniroyal Chemical Co., Inc., Middlebury, CT. (41313501)

Rice, F., B. Jacobson, and M.W. Winberry. 1989c. Terrestrial field dissipation for PCNB in potatoes. Uniroyal Project No. 8754C. Unpublished study performed by Agricultural Division Hill Hall of University of Minnesota, Crookston, MN, and Analytical Bio-Chemistry Laboratories, Inc., Columbia, MO; and submitted by Uniroyal Chemical Co., Inc., Middlebury, CT. (41216402)

Teeter, D. 1988. Laboratory volatility from soil of PCNB. Laboratory Project ID ABC #36283. Unpublished study performed by Analytical Bio-Chemistry Laboratories, Columbia, MO, and submitted by Uniroyal Chemical Company, Middlebury, CT. (40580201)

5. REVIEWED BY:

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

Date: DEC 31 1990

6. APPROVED BY:

Emil Regelman
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EFGWB/EFED/OPP

Date: JAN 16 1991

7. CONCLUSIONS:

A. Hydrolysis (40972601)

Pentachloronitrobenzene (PCNB) did not hydrolyze in sterile aqueous buffered (pH 5, 7, and 9) solutions incubated in sealed ampules in the dark at 25°C for up to 30 days.

This study is acceptable and fulfills EPA Data Requirements for Registering Pesticides by providing information on the hydrolysis of ring-labeled [^{14}C]PCNB in sterile aqueous solutions buffered to pH 5, 7, and 9.

B. Aerobic Soil Metabolism (41203601)

This study cannot be used to fulfill the aerobic soil metabolism data requirement.

This study is unacceptable for the following reasons:

a. The kinetics of the degradation of PCNB in soil was not adequately defined. The degradation rate data provided was assumed by the registrant to follow first-order kinetics, however, an r^2 value of 0.85 was calculated, indicating that the data cannot be explained using the first-order equation.

The registrant calculated a half-life of 80.2 days, however, upon examination of the data, this half-life value is not supported by the results which show an initial ^{14}C-PCNB concentration of ≈18.5 ppm in soil on day 0 and a concentration of 8.75 ppm after 30 days.

b. Residue identification was incomplete. Unidentified extractable ^{14}C-residues were observed at the TLC origin throughout the study. These residues increased from an average day-0 level of 0.09 ppm to a maximum of 2.16 ppm at 4 months posttreatment.

c. Characterization of the test samples was performed using only one-dimensional TLC and a single solvent system. This approach does not confirm the identity of residues. Although GC-MS is preferred whenever feasible, HPLC and then 2-dimensional TLC may prove to be acceptable if the HPLC and TLC systems employ different mobile phases and the separations achieved are unequivocal.

d. In the representative chromatogram that was submitted, a small peak was identified as PCP; however, a peak of approximately the same size was not identified; the study authors did not explain why the second peak was not identified (Figure 4).

Pentachloronitrobenzene (PCNB) dissipated with an observed half-life of 14 to 30 days from sandy loam soil incubated in the dark at 25°C. Nonvolatile degradates present in the soil were pentachloroaniline (PCA), pentachlorothioanisole (PCTA), and pentachlorophenol (PCP). Volatilized degradates included PCNB, PCA, PCTA, pentachlorobenzene (PCB), hexachlorobenzene (HCB), and carbon dioxide.

C. Aerobic Soil Metabolism (41384501)

This study cannot be used to fulfill the aerobic soil metabolism data requirement.

This study is **unacceptable** for the following reasons:

a. Residue identification was incomplete. Unidentified extractable ^{14}C-residues were observed at the TLC origin throughout the study. These residues increased from an average day-0 level of 0.16 ppm in soil to a maximum of 0.64 ppm at 122 days posttreatment.

b. The analytical methodology employed to separate and identify residues was insufficient. In this study, one-dimensional TLC with either one of two solvent systems was used to identify residues. Because TLC does not give confirmatory residue identification, HPLC was also employed, however, this only tentatively confirmed the presence of parent PCNB. HPLC did not give confirmatory identification of any degradates.

   Although GC-MS is preferred whenever feasible, HPLC and then 2-dimensional TLC may prove to be acceptable if the HPLC and TLC systems employ different mobile phases and the separations achieved are unequivocal.

c. The soil extracts were stored frozen prior to TLC and HPLC analyses. Examination of HPLC data in Appendix I revealed that the analyses were performed 5-9 months after the sampling date. Freezer storage stability data for PCNB and its degradates in soil extracts were not provided.

Pentachloronitrobenzene (PCNB) dissipated with a half-life of 77 days from sandy loam soil that was incubated in the dark at approximately 25°C. The major degradate was pentachloroaniline (PCA), and the degradate pentachlorothioanisole (PCTA) was also isolated. Volatilized residues included PCNB, PCA, and carbon dioxide.

D. Anaerobic Soil Metabolism (41203602)

This study cannot be used to fulfill the anaerobic soil metabolism data requirement.

This study is **unacceptable** for the following reasons:

a. Up to 17% of the [^{14}C]residues extracted from the soil (3 $\mu g/g$) and up to 67% of the residues in the flood water (0.4 $\mu g/g$) were not accounted for. The study authors did not specify whether these missing residues were unidentified degradates isolated on the TLC plates or were indistinguishable from background noise.

b. The analytical methodology employed to separate and identify residues was insufficient. In this study, one-dimensional TLC with one solvent system was used to identify non-volatile residues and GC was employed to identify volatiles. Neither method provides confirmatory identification. Although GC-MS is preferred whenever feasible, HPLC and then 2-dimensional TLC may prove to be acceptable if the HPLC and

TLC systems employ different mobile phases and the separations achieved are unequivocal.

c. The soil extracts and flood water were stored frozen for an unspecified period of time prior to TLC analysis. Freezer storage stability data for PCNB and its degradates in soil extracts and flood water were not provided.

Pentachloronitrobenzene (PCNB) dissipated under anaerobic conditions with an observed half-life of <30 days from sandy loam soil incubated in the dark at 25°C. Prior to establishing anaerobic conditions, the soil samples were incubated aerobically at a soil moisture of 75% of field capacity for 30 days. Nonvolatile degradates identified were pentachloroaniline (PCA), pentachlorothioanisole (PCTA), and pentachlorophenol (PCP). Volatilized residues included PCNB, PCA, PCTA, pentachlorobenzene (PCB), hexachlorobenzene (HCB), and carbon dioxide.

E. Laboratory Volatility (40580201)

This study cannot be used to fulfill the Laboratory Volatility data requirement.

This study is unacceptable for the following reasons:

a. The soil was not analyzed for PCNB residues; therefore, the application rate was not verified and material balances were not determined.

b. The soil was autoclaved before the test. Autoclaving of soils may significantly change the physical and chemical properties of the soils which may affect the adsorption of pesticides by the soils. Autoclaving may cause the soil to become more hydrophobic, or the soil CEC may change as a result of the breakdown of organic matter and/or the expansion of the crystalline structure of the clay particles. How autoclaving affected PCNB volatilization from this soil is unknown.

Less than 1% of the pentachloronitrobenzene (PCNB, 75% WP) applied to moist (25, 50, or 75% of field capacity) sterile sandy loam soil at a nominal concentration of 43 ppm was volatilized from the soil during 6.9 to 7.7 days of incubation in the dark at 25 ± 1°C. During the study, air flow through the experimental system varied between 71 and 281 mL/min.

The calculated vapor pressure of PCNB varied from 4.2×10^{-6} to 5.7×10^{-5} mm Hg, the volatility ranged from 4.9×10^{-4} to 1.5×10^{-2} $\mu g/cm^2 \cdot hr$, and the vapor density ranged from 77 to 200 $\mu g/m^3$.

F. Laboratory Volatility (41178001)

The volatility of pentachloronitrobenzene (PCNB) from sandy loam soil incubated in the dark at 50 or 75% of field moisture capacity and 25°C, ranged from 0.0622 to 0.171 $\mu g/cm^2/hr$. The calculated vapor pressure ranged from 3.14×10^{-5} mmHg to 8.19×10^{-5} mmHg and the vapor density ranged from 4.99×10^{-4} to 1.30×10^{-3} g/m^3. At 7 days posttreatment, volatilized PCNB residues totaled 1556-1650 μg (approximately 80% of the applied). Air flow through the system was 283-311 mL/min. PCNB was the

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only volatile residue found. During the study, material balances ranged from 90.3 to 111% of the applied.

This study is acceptable and fulfills EPA Data Requirements for Registering Pesticides by providing information on the volatility of pentachloronitrobenzene under laboratory conditions.

G. Field Dissipation - Terrestrial (41210501)

This study cannot be used to fulfill the Soil Field Dissipation data requirement.

This study is unacceptable for the following reasons:

a. The declared application rate (32.7 lb ai/A) was not confirmed by the soil samples taken immediately posttreatment or 1 day posttreatment. An application rate of 32.7 lb ai/A is equivalent to approximately 16 ppm in a 6-inch soil core. However, residues in the 0-6 inch soil sample measured only 6.2 ppm immediately posttreatment and 8.5 ppm 1-day posttreatment. No explanation was given for this discrepancy.

b. The grass was mowed 2 days after the first application. Since an unknown amount of PCNB would still be on the grass clippings and these clippings were either bagged or possibly blown off site (not specified in the report), the data cannot be used to accurately assess the dissipation of PCNB. This mowing may also explain the significant decrease in measured residues found on day 3 posttreatment as compared to those recorded on day 1 (3.6 ppm and 8.5 ppm, respectively).

c. Only 3 soil cores were sampled per sampling interval. This degree of replication is insufficient. A minimum of 15 soil cores with a minimum of three composites must be taken per sampling interval at each plot.

d. Residues were identified using only gas chromatography. This approach does not give confirmatory identification. Although GC-MS is preferred whenever feasible, GC or HPLC and then 2-dimensional TLC may prove to be acceptable if the HPLC and TLC systems employ different mobile phases and the separations achieved are unequivocal.

e. The registrant-calculated half-life of 35 days was determined based upon the second application being day 0. However, the sampling intervals were inadequate to define this half-life. The soil was not sampled until 32 days after the second treatment.

f. Daily rainfall and air temperature data were not provided, only monthly summaries. Soil temperature data were not provided.

g. Although frozen storage stability data were provided by the registrant, the study authors did not report how long the soil samples were stored frozen prior to analysis; therefore, the results of this field dissipation experiment could not be integrated with the available stability data.

h. Data from the control plot were not provided.

PCNB dissipated with a half-life of 35 days from the upper 6 inches of a Bermuda grass turf plot of sandy loam soil in California following the second of two treatments (33-day interval) of PCNB (Terraclor, 75% WP) at 1.0 lb of formulation/1000 feet^2/treatment (32.7 lb ai/A; which is the maximum label rate). The degradates pentachloroaniline, pentachlorothioanisole, and pentachlorobenzene were detected in the 0- to 6-inch soil layer up to 360 days posttreatment. Hexachlorobenzene was detected in the 0- to 6- inch soil layer up to 179 days posttreatment. PCNB and its degradates did not appear to leach below the 6-inch depth.

H. Field Dissipation - Terrestrial (41216401)

This study cannot be used to fulfill the Soil Field Dissipation data requirement.

This study is **unacceptable** for the following reasons:

a. The submitted freezer storage stability data indicate that many of the test samples were stored for longer than what the stability data permits before significant degradation takes place. The storage stability data supports a 120-day storage interval for PCNB, but only a 30-day interval for the metabolite PCB and the contaminant HCB. After this period of time, significant degradation was apparent. Many field test samples were stored for a period in excess of 120 days. The result of this excessive storage interval surely compromised the validity of the study.

b. The application rate was not confirmed by the immediately post-application residue measurement. At an application rate of 30 lbs ai/acre, there should have been ≈15.0 ppm in the soil (6-inch depth). However, the post-application sampling interval showed only 4.7 ppm and day 1 posttreatment measured only 7.7 ppm (the maximum level found throughout the study). The authors suggest that the volatility of PCNB may explain this loss, however, considering that the product was incorporated 4-6 inches into the soil immediately after treatment, their suggestion does not seem to account for a loss of ≈50% of the applied PCNB.

c. Residues were identified using only gas chromatography. This approach does not give confirmatory identification. Although GC-MS is preferred whenever feasible, GC or HPLC and then 2-dimensional TLC may prove to be acceptable if the HPLC and TLC systems employ different mobile phases and the separations achieved are unequivocal.

Pentachloronitrobenzene (PCNB) dissipated with a registrant-calculated half-life of 128 days from the upper 6 inches of a field plot of loamy sand soil in California treated with PCNB (Terraclor, 75% WP) at 30 lb ai/A. In the 0- to 6-inch soil depth, the average PCNB concentration was 4.3 ppm immediately posttreatment, increased to 6.9 ppm (maximum 9.9 ppm) at 1 day posttreatment, decreased to 2.7 ppm at 28 days, ranged from 1.9 to 3.8 ppm between 56 and 126 days, and declined to 0.30 ppm at 543 days. In the 0- to 6-inch soil depth, the degradate pentachlorobenzene (PCB) reached an average maximum concentration of 0.20 ppm at 56 days posttreatment; pentachlorothioanisole (PCTA) was a

maximum of 0.40 ppm at 28 days; pentachloroaniline (PCA) was a maximum of 0.94 ppm at 455 days; and hexachlorobenzene (HCB) was a maximum of 0.056 ppm at 543 days. At lower soil depths, PCNB was detected in the 6- to 12-inch soil layer at 0.0063 ppm immediately posttreatment, 0.0058 ppm at 7 days, and 0.0056 ppm at 126 days; PCNB was not detected (<0.005 ppm) at other sampling intervals. In the 12-to 18-inch soil layer, PCNB was not detected; however, in the 18- to 24-inch soil layer, PCNB was detected at two sampling intervals (0.0083 ppm at 7 days posttreatment and 0.056 ppm at 182 days). In the 6- to 12-inch soil layer, the degradate PCB increased to 0.015 ppm by 543 days posttreatment; PCTA, PCA, and HCB were not detected (<0.005 ppm). PCNB degradates were not detected in the 12- to 18-inch soil layer. In the 18-to 24-inch soil layer, PCA and PCTA were detected at one sampling interval (182 days posttreatment) at 0.023 and 0.0084 ppm, respectively; PCB and HCB were not detected at this depth.

I. Field Dissipation - Terrestrial (41216402)

This study cannot be used to fulfill the Soil Field Dissipation data requirement.

This study is unacceptable for the following reasons:

a. The application rate was not confirmed by the immediately post-application residue measurement. At an application rate of 25 lbs ai/acre, there should have been ≈12.5 ppm in the soil (6-inch depth). However, the post-application sampling interval showed only 4.2 ppm. The authors suggest that the volatility of PCNB may explain this loss, however, considering that the product was incorporated 4-6 inches into the soil immediately after treatment, their suggestion does not seem to account for a loss of >50% of the applied PCNB.

b. Residues were identified using only gas chromatography. This approach does not give confirmatory identification. Although GC-MS is preferred whenever feasible, GC or HPLC and then 2-dimensional TLC may prove to be acceptable if the HPLC and TLC systems employ different mobile phases and the separations achieved are unequivocal.

c. The submitted freezer storage stability data indicate that many of the test samples were stored for longer than what the stability data permits before significant degradation takes place. The storage stability data supports a 45-day storage interval for PCB. After this period of time, significant degradation was apparent. Many field test samples were stored for a period in excess of 60 days. The result of this storage interval surely compromised the validity of the study. In addition, the freezer storage stability data for HCB was highly variable and greater than 100% for eight of the thirteen sampling days (67-144%).

d. The variability in the data was such that the dissipation of PCNB could not be adequately explained using first-order kinetics. The r^2 value for the dissipation of PCNB in the 0-6" layer using first-order kinetics was a poor 0.83.

Pentachloronitrobenzene (PCNB) dissipated with a registrant-calculated half-life of 193 days from the upper 6 inches of a field plot of sandy loam soil in Minnesota treated with PCNB (Terraclor, 2 lb/gallon EC) at

25 lb ai/A. In the 0- to 6-inch soil depth, the average PCNB concentration was 4.1 ppm immediately posttreatment, was 3.2 ppm at 7 days, increased to 5.8 ppm at 14 days, decreased to 2.0 ppm by 298 days, and was 0.67 ppm at 546 days. In the 0-to 6-inch soil depth, the degradates pentachloroaniline (PCA) and pentachlorobenzene (PCB) gradually reached maximum concentrations of 1.1 and 0.18 ppm, respectively, by 546 days posttreatment. Pentachlorothioanisole (PCTA) was a maximum of 0.12 ppm at 56 days; and hexachlorobenzene (HCB) was a maximum of 0.025 ppm at 56-84 days. At lower soil depths, PCNB was detected in the 6- to 12-inch soil layer at 0.010-0.011 ppm at 1-14 days posttreatment and at 0.0077 ppm at 126 days; PCNB was not detected (<0.005 ppm) at other sampling intervals. In the 12- to 18-inch soil layer, PCNB was 0.0067 ppm immediately posttreatment, 0.032 ppm at 28 days, and 0.009 ppm at 56 days; and in the 18- to 24-inch soil layer, PCNB was at 0.0076-0.021 ppm at 7-84 days and 0.0067 ppm at 298 days. The degradate PCB was detected at 0.072-0.011 ppm at 1 and 14 days posttreatment in the 6- to 12- and 12- to 18-inch soil depths, and at 0.010 ppm at 14 days in the 18- to 24-inch depth. PCA was detected at 0.0071 ppm at 126 days in the 6- to 12-inch depth, was not detected (<0.005 ppm) in the 12- to 18-inch depth, and was detected at 0.011 ppm at 298 days in the 18- to 24-inch depth. PCTA and HCB were not detected (<0.005 ppm) at any depth below 6 inches.

J. Field Dissipation - Terrestrial (41313501) **From EFGWB review dated 6/27/90**

This study is not acceptable in fulfilling the Soil Field Dissipation data requirement. The following deficiencies were noted:

a. Measured residues detected in the 0-6", 6-12", 12-18", and 18-24" soil cores were extremely erratic. Concentrations increased and decreased with no apparent pattern. For example, the total residue as parent found in the 0-6" layer was measured at 3.7 ppm on day 1, 0.28 ppm on day 7, 0.70 ppm on day 14, 0.094 ppm on day 27 and 0.66 ppm on day 127. This inconsistent pattern was also seen in the 6-12" and 12-18" layers. The authors attribute the variability in the data to the result of a heavy thunderstorm which occurred immediately following the application, where run-off to low areas may have occurred, thus concentrating the PCNB. The variability was also attributed to contamination during sampling.

Although the two reasons given above may indeed have led to the extreme variability in the data, this rationale cannot suffice for reliable data that is scientifically sound. The exceptionally poor r^2 values (0.32, 0.25, and 0.24 for 0-6" PCNB, 0-6" total residue, and 0-24" total residue, respectively) for the dissipation curves prohibit making any convincing conclusions about the dissipation of PCNB and the formation and dissipation of its degradates based upon first-order kinetics.

b. The submitted freezer storage stability data indicate that many of the test samples were stored for longer than what the stability data permits before significant degradation takes place. The storage stability data supports a 120-day storage interval when PCNB is concerned, but only a 30-day interval when the metabolite, PCB and the contaminant HCB, are concerned. After this period of time, significant degradation was apparent. Many field test samples were

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stored for a period in excess of 90 days (average: 102 days). The result of this excessive storage interval surely compromised the validity of the study.

c. In addition to the 0.5 inches of irrigation immediately after application to wash the granules off the foliage, there was a severe 0.27 inch thunderstorm shortly after that and 0.55 inches of rain on day 2. All of this precipitation may have washed much of the granular pesticide from the intended application site. It appears from the exceedingly variable results that these rainfall events served to essentially ruin any hopes of collecting meaningful data for the evaluation of mobility, degradation, and dissipation of residues. Perhaps the study should have been discontinued after these unfortunate rainfall events.

d. Residues were identified using only gas chromatography. This approach does not confirm the identity of residues. Although GC-MS is preferred whenever feasible, GC or HPLC and then 2-dimensional TLC may prove to be acceptable if the HPLC and TLC systems employ different mobile phases and the separations achieved are unequivocal.

e. The application rate was not confirmed by the immediately post-application residue measurement. At an application rate of 10 lbs ai/acre, there should have been ≈5.0 ppm in the soil at a 6-inch depth. However, the post-application sampling interval showed only 3.7 ppm. This may have been due to run-off from the thunderstorm which occurred shortly after application, in addition to the fact that the post-application sample was not taken until the next day.

Terraclor (PCNB) formulated as a 10% granule (10G) was applied to peanuts at a site near Donalsonville, Georgia. The soil was a sandy loam with 1.9% organic matter, 4.8 pH, 2.2 meq/100 g CEC, and a 1.38 g/cc bulk density. A single application of PCNB was made at the rate of 100 pounds of Terraclor 10G per 12,400 linear feet of row (maximum application rate according to product label). The study area received 0.5 inches of irrigation immediately after the application to wash the granules from the plants and help dissolve and immobilize the compound.

The dissipation half-life of PCNB in the 0-6" layer was 116 days indicating a slow breakdown into metabolites. Only very low levels of PCNB residues at 6-12", 12-18" and 18-24" were detected. The metabolite PCA was detected in the 0-6" layer at every sampling date during the study. Detected residues increased to Day 465 but accumulation was erratic. The metabolites PCB and PCTA appeared in the 0-6" layer after Day 27 through Day 465. The contaminant HCB was detected early but was below the detection limit (0.005 ppm), after Day 27. The metabolites and contaminant were detected at some depths below the 0-6" layer at very low levels.

The dissipation half-life of the total residue (the sum of PCNB, PCA, PCTA, PCB, and HCB) was 193 days in the 0-6" layer. When the 0-6", 6-12", 12-18", and 18-24" depths were considered together, the dissipation half-life of the total residue changed slightly to 202 days.

K. Confined Accumulation - Rotational Crops (41562905)

This study cannot be used to fulfill the Confined Accumulation in Rotational Crops data requirement at this time.

This study is not acceptable for the following reasons:

a. The PCNB residues in the plant tissue and soil samples were not characterized. The samples were analyzed only for total radioactive residues.

b. The length of freezer storage of crop and soil samples prior to analysis was not reported, and no freezer storage stability data were provided.

c. Material balances and supporting raw data were not provided.

d. The application rate was not confirmed by the immediately post-application residue measurement. At an application rate of 30 lbs ai/acre, there should have been ≈15 ppm in the soil (6-inch depth). However, the 2-hour post-application sampling showed that none of the plots reached 15 ppm in the soil and many of them measured below 10 ppm.

Uncharacterized [^{14}C]pentachloronitrobenzene (PCNB) residues accumulated in lettuce, turnips, and wheat that were planted in sheltered outdoor plots of fine sandy loam soil at 30, 120, and 365 days after the soil was treated with [^{14}C]PCNB (radiochemical purity 100%) plus unlabelled PCNB (purity 99.2%) at 30 lb ai/A.

In immature wheat, PCNB residues were 2.59 and 5.05 ppm in wheat planted at 30 and 365 days posttreatment, respectively. In the mature wheat straw, PCNB residues were 22.2-25.9 ppm; in the mature wheat hulls, PCNB residues were 6.06-11.1 ppm; and in the grain, PCNB residues were 0.332-0.710 ppm.

In immature turnips, PCNB residues were 4.61 and 1.60 ppm in turnips planted at 30 and 365 days posttreatment, respectively. In mature turnip greens, PCNB residues were 3.63 ppm in turnips planted at 30 days posttreatment and 0.727 ppm in turnips planted at 365 days. In mature turnip roots, PCNB residues were 20.3 ppm in turnips planted at 30 days posttreatment and 1.48 ppm in turnips planted at 365 days.

In immature lettuce, PCNB residues were 1.40-5.67 ppm. In mature lettuce PCNB residues were 0.146-1.62 ppm.

In the upper 6 inches of the soil, uncharacterized PCNB residues were 6.56-14.3 ppm at 2 hours posttreatment, 8.41-12.6 ppm at 30 days, 5.89-8.02 ppm at 120 days, 4.84-6.52 ppm at 365 days, and 4.84-5.61 ppm at 426-472 days. PCNB residues were sporadically recovered at 0.024-1.05 ppm in the 6- to 12-inch soil layer.

Although ^{14}C-residues were found in all three crops planted 30, 120, and 365 days posttreatment; because these residues were not characterized, a Field Accumulation in Rotational Crops study would not be appropriate at this time. The authors stated that residue analysis was in progress. Confirmatory residue identification, material balances, and storage stability data must be submitted for this study. Once these data are submitted and if found acceptable, then a decision can be made to either conduct a Field Accumulation study for the purpose of setting a rotational interval or, petition for tolerances. If the supporting data are not found to be acceptable, a new confined accumulation study will be required.

L. Laboratory Accumulation - Fish (40580202)

This study cannot be used to fulfill the Bioaccumulation in Fish data requirement at this time.

This study is scientifically sound and provides supplemental information, but does not meet Subdivision N guidelines for the following reason:

a. Radioactive residues in the water and fish tissues were not characterized. Fish samples were collected on days 21 and 28 of exposure and on day 14 of depuration for "metabolite characterization", but the results of these analyses were not presented in this study.

Uncharacterized pentachloronitrobenzene (PCNB) residues accumulated in bluegill sunfish exposed to [^{14}C]PCNB at a mean concentration of 0.54 ppb for 28 days. Maximum mean bioconcentration factors were 370x for edible tissues, 1800x for viscera, and 960x for whole fish. At the end of the 21-day depuration period, 81-84% of the accumulated [^{14}C]residues were eliminated from the fish tissues.

In order for this study to fulfill the accumulation in laboratory fish data requirement, data confirming the identification of PCNB residues in the water and fish tissues and supporting storage stability data must be submitted.

M. Field Accumulation - Aquatic Nontarget Organisms (41521001)

This study is not acceptable for the following reasons:

a. Residues in the fish tissues, water, and soil were not characterized.

b. At 28 days posttreatment, approximately 29% of the applied radioactivity was unaccounted for.

Uncharacterized pentachloronitrobenzene (PCNB) residues accumulated in channel catfish and bluegill sunfish maintained under simulated field conditions for 28 days in water treated with a single application of PCNB at 0.10 ppm. The maximum mean bioconcentration factors for channel catfish were 250x in the edible tissues, 630x in the visceral tissues, and 460x in the whole fish; the maximum mean bioconcentration factors for bluegill sunfish were 120x in the edible tissues, 560x in the visceral tissues, and 330x in the whole fish.

The PCNB Registration Standard (January 1987), inadvertently required an Accumulation in Aquatic Non-Target Organisms study. However, under the presently registered uses of PCNB (terrestrial food and non-food), this study is not required. The Ecological Effects Branch of EFED was consulted on this matter, (Allen Vaughan, 1/5/88), and their conclusions were in agreement with those of EFGWB. Although PCNB does bioconcentrate in fish tissue, there is appreciable depuration. At the present time and with the currently registered uses, an Accumulation in Aquatic Non-Target Organisms study is not required.

ENVIRONMENTAL FATE ASSESSMENT:

Acceptable studies have shown that PCNB does not hydrolyze under sterile aqueous conditions at pH 5, 7 or 9 at 25°C, and it photodegrades very slowly ($t_{1/2}$: ≈80 days) on the surface of soil exposed to a filtered Xenon Arc light system. PCNB adsorbs to soil and is not likely to leach to ground water. The mobility of its degradates PCA, PCTA, PCB, and the contaminant HCB, has not been adequately defined. PCNB demonstrated significant volatilization from soil; at 7 days posttreatment, approximately 80% of the applied had volatilized from a sandy loam incubated at 25°C. The vapor pressure of PCNB is 1.13×10^{-4} mm Hg at 25°C. The metabolism of PCNB in soil under aerobic and anaerobic conditions is not well understood.

Several soil field dissipation studies have been conducted, however, none have been found to be acceptable. These studies do indicate that PCNB tends to remain in the 0-6 inch layer and that it is persistent. Half-lives in the 0-6 inch layer were: 35 days in a sandy loam turf plot in California; 128 days in a loamy sand soil in California planted with broccoli; 193 days in a sandy loam potato plot in Minnesota; and 116 days in a sandy loam peanut plot in Georgia. PCTA, PCA, PCB, and HCB were also persistent in these studies. These residues were detected sporadically at depths below the 0-6 inch layer at low concentrations, however, it was not clear from the data whether there was actual leaching through the soil profile or if there was a contamination problem during sampling.

Although the study was not acceptable, the data from a confined accumulation in rotational crops study did demonstrate that leafy vegetables, root crops, and small grains accumulate significant amounts of PCNB residues (yet to be identified) even after being planted 12 months posttreatment. Some examples of the level of residues found in crops planted 12 months after application of PCNB are: 0.61 ppm in mature lettuce, 1.5 ppm in turnip roots, 25.9 ppm in wheat straw, 8.0 ppm in wheat hulls, and 0.38 ppm in wheat grain.

PCNB also accumulates in fish. An accumulation in fish study demonstrated that PCNB residues (yet to be defined) bioconcentrate in the tissues of bluegill sunfish. BCF's were 370x, 1800x, and 960x for edible, viscera, and whole fish, respectively. However, after the 21-day depuration period, 81-84% of the accumulated residues were eliminated from the fish tissues.

In summary, PCNB is expected to be persistent in the environment. The degradates PCA, PCTA, PCB and the contaminant HCB are also persistent. PCNB is somewhat immobile in soil and is not likely to leach to ground water, however, the potential for its degradates to leach has not been clearly defined. PCNB is moderately volatile and may dissipate through volatilization unless measures such as soil incorporation are taken. There is a tendency for residues of PCNB to accumulate in crops rotated several months after application and also to bioaccumulate in fish.

8. RECOMMENDATIONS:

The fate of PCNB and its degradates, particularly metabolism in soil and dissipation under field conditions, is not yet well understood. The studies that must be conducted to fulfill the remaining data gaps are summarized below. (Because there are two registrants generating data independently in response to the registration standard, a separate list of data requirements has been generated for each company).

UNIROYAL CHEMICAL CO.

SATISFIED

Hydrolysis 161-1 (40972601)
Leaching-Adsorption/Desorption 163-1 (00114168, 00114181)

NOT SATISFIED

Photodegradation in Water 161-2
Photodegradation in Soil 161-3
Aerobic Soil Metabolism 162-1
Anaerobic Soil Metabolism 162-2
Laboratory Volatility 163-2
Field Volatility 163-3
Soil Field Dissipation 164-1
Confined Accumulation in Rotational Crops 165-1
Accumulation in Fish 165-4

RESERVED

Long-Term Soil Field Dissipation 164-5
Field Accumulation in Rotational Crops 165-2

AMVAC CHEMICAL CORP.

SATISFIED

Hydrolysis 161-1 (40865301)
Photodegradation on Soil 161-3 (41004801)
Laboratory Volatility 163-2 (41178001)

NOT SATISFIED

Photodegradation in Water 161-2
Aerobic Soil Metabolism 162-1
Anaerobic Soil Metabolism 162-2
Leaching-Adsorption/Desorption 163-1
Field Volatility 163-3
Soil Field Dissipation 164-1
Confined Accumulation in Rotational Crops 165-1
Accumulation in Fish 165-4

RESERVED

Long-Term Soil Field Dissipation 164-5
Field Accumulation in Rotational Crops 165-2

The 1987 PCNB Registration Standard imposed an interim prohibition against rotating root crops for 12 months after broadcast and banding applications because of preliminary data to indicate that peanuts may bear detectable residues of PCNB when planted in rotation with a broadcast application made eight months earlier. However, there were no data at the time to prohibit the rotation of non-root crops following broadcast treatment or root crops following either seed or transplant treatment with PCNB.

The confined rotational crop study reviewed in this package indicates that PCNB residues remain in the soil for over 12 months and are accumulated by non-root crops as well as root crops that are planted 12 months after treatment. It is, therefore, recommended that an interim restriction be imposed against rotating to any crop for 12 months after an application (other than seed treatment), of PCNB unless a tolerance has been established for that crop. According to CFR 40 §180.319, an interim tolerance of 0.1 ppm has been established for PCNB in bananas, beans, broccoli, brussels sprouts, cabbage, cauliflower, garlic, peppers, potatoes, and tomatoes. Also, an interim tolerance of 1.0 ppm has been established for peanuts. The extent of the restriction should be reconsidered when additional data are submitted and reviewed.

9. BACKGROUND:

PCNB (pentachloronitrobenzene) is a fungicide registered for use on a variety of terrestrial food crop (field and vegetable) and terrestrial nonfood (ornamentals and turf) use sites. Single active ingredient formulations consist of 10-40% D, 75% WP, 2-30% G, 23.4-26.5% EC, 20% FlC, and 20-25% RTU-L. PCNB may be formulated with several compounds including fenaminosulf, thiram, captan, truban, carbaryl, disulfoton, phorate, cycloheximide, malathion, and carboxin. Application rates range from 0.025-3.0 lb/100 lb seed for seed treatment, 1.4-4.5 lb/100 gal for transplant solutions, 0.75-1.5 lb/100 gal for storage treatment (roses), 0.25-2.27 lb/A or 0.2-0.3 lb/gal for soil applications, and 0.422-0.562 lb/100 gal or 0.035-1.0 lb/1000 ft^2 for foliar applications. PCNB is generally used as a seed treatment, a spray using ground equipment, or a granular soil application.

10. DISCUSSION OF INDIVIDUAL TESTS OR STUDIES:

See individual DER's.

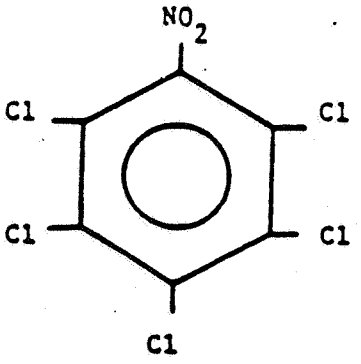
11. COMPLETION OF ONE-LINER:

Amended as applicable.

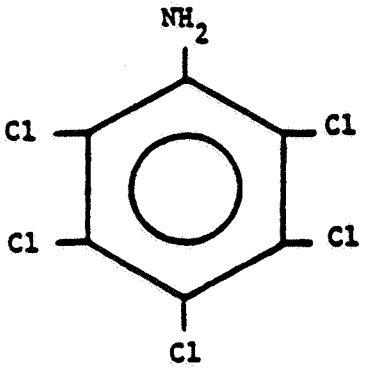
12. CBI APPENDIX:

Not applicable.

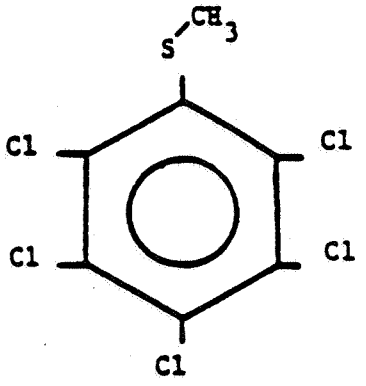
Chemical Structures of PCNB, PCA, PCTA, PCB and HCB



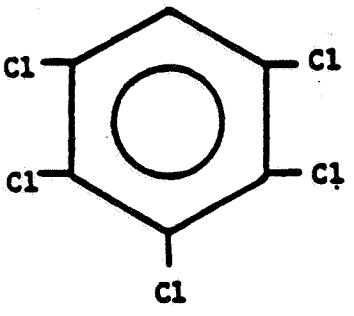
PCNB (Pentachloronitrobenzene)



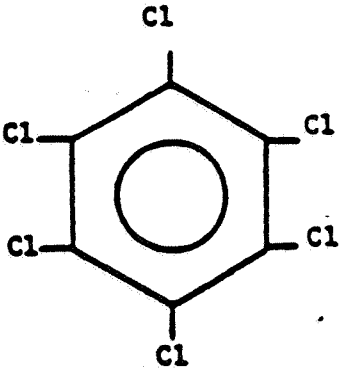
PCA (Pentachloroaniline)



PCTA (Pentachlorothioanisole)



PCB (Pentachlorobenzene)



HCB (Hexachlorobenzene)

PCNB

Table of Contents

DATA EVALUATION RECORD

STUDY 1

CHEM 056502 Pentachloronitrobenzene §161-1

FORMULATION--00--ACTIVE INGREDIENT

STUDY ID 40972601
Bowman, B.R., and M. Fennessey. 1988. Determination of the hydrolysis rate of ^{14}C-PCNB. ABC Final Report No. 36005. Unpublished study performed by Analytical Bio-Chemistry Laboratories, Inc., Columbia, MO, and submitted by Uniroyal Chemical Company, Inc., Middlebury, CT.

DIRECT REVIEW TIME = 12

REVIEWED BY: C. Little TITLE: Staff Scientist

EDITED BY: T. Colvin-Snyder TITLE: Staff Scientist
K. Patten Task Leader

APPROVED BY: W. Spangler TITLE: Project Manager

ORG: Dynamac Corporation
Rockville, MD
TEL: 468-2500

SECONDARY REVIEW BY: D. Spatz
TITLE: Chemist
ORG: EFGWB/EFED/OPP

SIGNATURE: DEC 28 1990

CONCLUSIONS:

Degradation - Hydrolysis

1. This study can be used to fulfill the Hydrolysis data requirement.

2. Pentachloronitrobenzene (PCNB) did not hydrolyze in sterile aqueous buffered (pH 5, 7, and 9) solutions incubated in sealed ampules in the dark at 25°C for up to 30 days.

3. This study is acceptable and fulfills EPA Data Requirements for Registering Pesticides by providing information on the hydrolysis of ring-labeled [^{14}C]PCNB in sterile aqueous solutions buffered to pH 5, 7, and 9.

METHODOLOGY:

Uniformly ring-labeled [^{14}C]pentachloronitrobenzene (radiochemical purity 98.6%, specific activity 8.9 mCi/mmol, Uniroyal), in acetonitrile, was added at a nominal concentration of 0.3 μg/ml to flasks containing sterile aqueous solutions buffered to pH 5 (0.2 M acetate), pH 7 (0.01 M HEPES), pH 7 (0.2 M tris), and pH 9 (0.2 M borate). The final concentration of the acetonitrile cosolvent in the test solutions was <1%. The treated solutions were mixed by sonication for at least 15 minutes. Aliquots of each test solution were placed in ampules, which were then flame-sealed and incubated in the dark at 25 ± 1°C for up to 30 days. Duplicate ampules were collected for analysis at 0, 1, 13, and 30 days posttreatment.

On the day of sampling, each ampule was frozen using a dry ice/acetone bath. The ampule was then broken open, hexane (1 mL) was added to the ampule, and the contents of the ampule were allowed to thaw. The ampule solution was then transferred to a culture tube and shaken, and the hexane layer was transferred to a separate flask using a pipette. The empty ampule was rinsed twice with hexane. After each rinsing, the hexane was added to the aqueous solution in the culture tube and used as an extraction solvent. The hexane extracts were combined, and the extracts and extracted aqueous solution were stored frozen until further analysis. Duplicate aliquots of the extracts and aqueous solution were analyzed for total radioactivity by LSC. Aliquots of the hexane extracts from the 30-day sampling interval were analyzed by GC/MS in the electron impact mode.

DATA SUMMARY:

Uniformly ring-labeled [^{14}C]pentachloronitrobenzene (PCNB, radiochemical purity 98.6%), at 0.3 μg/mL, did not hydrolyze in sterile aqueous buffer (pH 5, 7, and 9) solutions incubated in sealed ampules in the dark at 25 ± 1°C for up to 30 days. At 30 days posttreatment, parent PCNB was the only compound present in the solutions. During the study, material balances ranged from 96 to 106% based on time 0 analysis.

COMMENTS:

1. Only test solutions sampled at 30 days posttreatment were analyzed by GC/MS. Test solutions sampled at other intervals were analyzed only for total radioactivity by LSC.

2. An initial study of the hydrolysis of PCNB in aqueous solution was performed prior to the definitive study described in this review. Data from the initial study were considered inadequate by the study authors due to the low material balances that were obtained.

Also, in the initial study, the degradate pentachloroaniline was detected in the pH 7 (HEPES and tris buffers) test solution; it was not, however, detected in any test solutions from the definitive study reviewed here. The study author stated that it was most likely that the results obtained in the initial study were due to incomplete sealing of the screw-cap containers, which could have resulted in volatilization of the parent compound and allowed for microbial contamination of the solutions.

PCNB environmental fate review

Page _____ is not included in this copy.

Pages 22 through 32 are not included in this copy.

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 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

X FIFRA registration data

___ The document is a duplicate of page(s) _____

___ The document is not responsive to the request

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.

DATA EVALUATION RECORD

STUDY 2

CHEM 056502 Pentachloronitrobenzene §162-1

FORMULATION--00--ACTIVE INGREDIENT

STUDY ID 41203601
Daly, D., and W. Cranor. 1989. Aerobic soil metabolism of ^{14}C-pentachloronitrobenzene. ABC Final Report No. 35904. Unpublished study performed by Analytical Bio-Chemistry Laboratories, Inc., Columbia, MO, and submitted by Uniroyal Chemical Company, Inc., Middlebury, CT.

DIRECT REVIEW TIME = 22

REVIEWED BY: C. Little TITLE: Staff Scientist

EDITED BY: T. Colvin-Snyder TITLE: Staff Scientist
K. Patten Task Leader

APPROVED BY: W. Spangler TITLE: Project Manager

ORG: Dynamac Corporation
Rockville, MD

SECONDARY REVIEW BY: D. Spatz
TITLE: Chemist
ORG: EFGWB/EFED/OPP

SIGNATURE: DEC 28 1990

CONCLUSIONS:

Metabolism - Aerobic Soil

1. This study cannot be used to fulfill the aerobic soil metabolism data requirement.

2. Pentachloronitrobenzene (PCNB) dissipated with an observed half-life of 14 to 30 days from sandy loam soil incubated in the dark at 25°C. Nonvolatile degradates present in the soil were pentachloroaniline (PCA), pentachlorothioanisole (PCTA), and pentachlorophenol (PCP). Volatilized degradates included PCNB, PCA, PCTA, pentachlorobenzene (PCB), hexachlorobenzene (HCB), and carbon dioxide.

3. This study is unacceptable for the following reasons:

a. The kinetics of the degradation of PCNB in soil was not adequately defined. The degradation rate data provided was assumed by the registrant to follow first-order kinetics, however, an r^2 value of 0.85 was calculated, indicating that the data cannot be explained using the first-order equation.

The registrant calculated a half-life of 80.2 days, however, upon examination of the data, this half-life value is not supported by the results which show an initial ^{14}C-PCNB concentration of ≈18.5 ppm in soil on day 0 and a concentration of 8.75 ppm after 30 days.

b. Residue identification was incomplete. Unidentified extractable ^{14}C-residues were observed at the TLC origin throughout the study. These residues increased from an average day-0 level of 0.09 ppm to a maximum of 2.16 ppm at 4 months posttreatment.

c. Characterization of the test samples was performed using only one-dimensional TLC and a single solvent system. This approach does not confirm the identity of residues. Although GC-MS is preferred whenever feasible, HPLC and then 2-dimensional TLC may prove to be acceptable if the HPLC and TLC systems employ different mobile phases and the separations achieved are unequivocal.

d. In the representative chromatogram that was submitted, a small peak was identified as PCP; however, a peak of approximately the same size was not identified; the study authors did not explain why the second peak was not identified (Figure 4).

METHODOLOGY:

Uniformly ring-labeled [^{14}C]pentachloronitrobenzene (PCNB; radiochemical purity >95%, specific activity 8.9 mCi/mmol, Uniroyal), in acetonitrile, was added at a nominal rate of 25 ppm to 30 culture tubes containing air-dried, sieved (2 mm) sandy loam soil (64% sand, 20% silt, 16% clay, organic matter 1.6%, pH 6.2, CEC 9.5 meq/100 g). An additional 16 soil samples were prepared to serve as controls. The culture tubes containing the treated soil were vortexed to ensure mixing, and deionized water was added to all tubes to bring the soil moisture content to 75% of field capacity. The soil samples (treated and control) were then placed in a 3000-mL resin pot that was connected, in series, to volatile traps of ethylene glycol, 1 N H_2SO_4, and 1 N potassium hydroxide (two traps) (Figure 2). A rubber extension plug fitted into the center hole of the resin pot allowed for removal of the individual culture tubes. The rate of air flow through the system was approximately 50 mL/min. The soil samples

were incubated in the dark at 25 ± 1°C. Samples were collected for analysis at 0, 1, 3, 7, 14, 30, 61, 92, 122, 183, 274, and 366 days posttreatment.

Soil samples from days 0 and 1 were extracted three times with methanol by shaking; subsequent samples were extracted four times with methanol:1 N acetic acid (80:20) by shaking. The soil:solution slurries were centrifuged and the extract was removed. Triplicate aliquots of the combined extracts were analyzed for total radioactivity by LSC. Extracts were stored frozen when not in use. The extracts were also cochromatographed with nonradiolabeled reference standards using TLC on silica gel plates developed with hexane:toluene:acetone (7:3:1, v:v:v). Radioactive zones on the plates were located and quantified using a radiochromatogram scanner; the zones were also visualized using autoradiography. Radioactive zones were identified by comparison with reference standards, which were visualized with UV light. Triplicate subsamples of the extracted soil were analyzed by LSC following combustion.

Each ethylene glycol trapping solution was partitioned three times with methylene chloride. Aliquots of the combined methylene chloride fraction were analyzed using LSC; the remaining methylene chloride was evaporated to dryness in a flask which was then rinsed with methanol. The methanol rinse was evaporated to dryness and reconstituted in methanol twice, then concentrated by partial evaporation. Aliquots of the concentrated methanol were analyzed by LSC and by GC with electron-capture detection. Trapping solutions from the H_2SO_4 and KOH volatile traps were analyzed for total radioactivity by LSC.

DATA SUMMARY:

Uniformly ring-labeled [^{14}C]pentachloronitrobenzene (PCNB; radiochemical purity >95%), at 20 ppm, dissipated with an observed half-life of 14 to 30 days from sandy loam soil incubated at 25 ± 1°C. In the soil, PCNB decreased from 18.58 ppm at day 0 to 8.75 ppm by 30 days posttreatment, and to 1.03 ppm by 366 days posttreatment. Degradates in the soil were

pentachloroaniline (PCA),

present at a maximum of 4.82 ppm PCNB equivalents at 9 months posttreatment;

pentachlorothioanisole (PCTA),

present at a maximum of 1.22 ppm PCNB equivalents at 1 day posttreatment; and

pentachlorophenol (PCP),

present at a maximum of 0.79 ppm PCNB equivalents at 366 days posttreatment. Extractable residues remaining at the TLC origin comprised a maximum of 2.16 ppm PCNB equivalents at 122 days posttreatment. Unextractable residues reached a maximum of 3.41 ppm PCNB equivalents at 274 days posttreatment.

At 366 days posttreatment, volatiles totaled 7.87 ppm PCNB equivalents. $^{14}CO_2$ comprised 2.4% of the total volatiles at 366 days posttreatment. Other volatiles were comprised mostly of PCNB and of smaller amounts of PCA, PCTA,

pentachlorobenzene (PCB), and

hexachlorobenzene (HCB).

Total recoveries ranged from 16.87 to 20.48 ppm PCNB equivalents.

COMMENTS:

1. The soil extracts were stored frozen for an unspecified period of time prior to TLC analysis. Freezer storage stability data for PCNB and its degradates in soil extracts were not provided.

PCNB environmental fate review

Page _____ is not included in this copy.

Pages 37 through 46 are not included in this copy.

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 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

X FIFRA registration data

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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.

DATA EVALUATION RECORD

STUDY 3

CHEM 056502 Pentachloronitrobenzene §162-1

FORMULATION--00--ACTIVE INGREDIENT

STUDY ID 41384501
Cranor, W. 1989. Aerobic soil metabolism of ^{14}C-pentachloronitrobenzene. ABC Final Report No. 36824. Unpublished study performed by Analytical Bio-Chemistry Laboratories, Inc., Columbia, MO, and submitted by AMVAC Chemical Corporation, Los Angeles, CA.

DIRECT REVIEW TIME = 12

REVIEWED BY: W. Hurtt TITLE: Staff Scientist

EDITED BY: T. Colvin-Snyder TITLE: Staff Scientist
K. Patten Task Leader

APPROVED BY: W. Spangler TITLE: Project Manager

ORG: Dynamac Corporation
Rockville, MD

SECONDARY REVIEW BY: D. Spatz
TITLE: Chemist
ORG: EFGWB/EFED/OPP

SIGNATURE: DEC 28 1990

CONCLUSIONS:

Metabolism - Aerobic Soil

1. This study cannot be used to fulfill the aerobic soil metabolism data requirement.

2. Pentachloronitrobenzene (PCNB) dissipated with a half-life of 77 days from sandy loam soil that was incubated in the dark at approximately 25°C. The major degradate was pentachloroaniline (PCA), and the degradate pentachlorothioanisole (PCTA) was also isolated. Volatilized residues included PCNB, PCA, and carbon dioxide.

3. This study is unacceptable for the following reasons:

   a. Residue identification was incomplete. Unidentified extractable ^{14}C-residues were observed at the TLC origin throughout the study. These residues increased from an average

day-0 level of 0.16 ppm in soil to a maximum of 0.64 ppm at 122 days posttreatment.

b. The analytical methodology employed to separate and identify residues was insufficient. In this study, one-dimensional TLC with either one of two solvent systems was used to identify residues. Because TLC does not give confirmatory residue identification, HPLC was also employed, however, this only tentatively confirmed the presence of parent PCNB. HPLC did not give confirmatory identification of any degradates.

Although GC-MS is preferred whenever feasible, HPLC and then 2-dimensional TLC may prove to be acceptable if the HPLC and TLC systems employ different mobile phases and the separations achieved are unequivocal.

c. The soil extracts were stored frozen prior to TLC and HPLC analyses. Examination of HPLC data in Appendix I revealed that the analyses were performed 5-9 months after the sampling date. Freezer storage stability data for PCNB and its degradates in soil extracts were not provided.

METHODOLOGY:

Air-dried, sieved (2 mm) sandy loam soil (54% sand, 36% silt, 10% clay, organic matter content 0.8%, pH 6.5, CEC 4.7 meq/100 g) was moistened and treated with uniformly ring-labeled [^{14}C]pentachloronitrobenzene (PCNB; radiochemical purity 98.6%, specific activity 46.4 mCi/mmol, Chemsyn Science Laboratories), dissolved in hexane, which was evaporated under a stream of nitrogen. Additional moistened soil was added, and the soil was mixed. The final concentration of PCNB was determined to be 10.467 μg/g by triplicate LSC analyses following combustion. Samples of treated soil were placed in test tubes, and deionized water was added to each tube to bring the soil to approximately 75% of field capacity. The tubes were placed within a metabolism chamber that was maintained under positive pressure by an air flow system that supplied humidified CO_2-free air at 50 mL/minute (Figure 2). Air exiting the chamber passed sequentially through tubes containing ethylene glycol, 1 N sulfuric acid, and 1 N KOH (two tubes). The moisture level of the soil was maintained at approximately 75% of field capacity by periodically adding deionized water to each sample; moisture adjustment intervals varied from 1 to 9 days for 3 months and then from 13 to 62 days for the remainder of the experiment. The samples within the metabolism chamber were maintained for up to 1 year in the dark at 25.3 $\pm$ 0.2°C. To serve as controls, test tubes of untreated soil were incubated in a duplicate system. Tubes of soil were removed for analysis at intervals up to 365 days posttreatment.

A portion of each soil sample was extracted three times with methanol:1 N acetic acid (80:20, v:v) followed by centrifugation. The extracts were combined and, after appropriate rinsing and

dilution with additional methanol:acetic acid solvent, triplicate aliquots of the extract were analyzed for total radioactivity by LSC. The remaining extract was stored in a freezer (temperature not reported) for an unspecified period of time prior to further analysis.
The ethylene glycol, sulfuric acid, and potassium hydroxide trapping solutions were analyzed for total radioactivity by LSC. Each ethylene glycol trapping solution was extracted four times with methylene chloride. Aliquots of the 3- through 122-day ethylene glycol trapping solutions were diluted with deionized water prior to extraction. The combined extracts were evaporated to dryness, dissolved in methanol, and analyzed in triplicate by LSC. Selected extracts were concentrated by evaporation under a stream of nitrogen and redissolved in methanol.

Extracts of the soils and ethylene glycol trapping solutions were analyzed by TLC and HPLC. For the TLC analysis, silica gel plates were developed either in hexane or hexane:toluene:acetone (7:3:1, v:v:v). The samples were cochromatographed with reference standards of PCNB, pentachloroaniline (PCA), pentachlorothioanisole (PCTA), pentachlorobenzene (PCB), 2,3,4,5-tetrachloronitrobenzene (2,3,4,5-TCNB), 2,3,5,6-tetrachloronitrobenzene (2,3,5,6-TCNB), and hexachlorobenzene (HCB). After development, radioactive areas on the plates were located and quantified using a radiochromatogram scanner. In addition, the 0- and 14-day plates were autoradiographed and analyzed by LSC. For the HPLC analysis, aliquots from selected samples were analyzed using a C-18 column and a gradient system of acetonitrile and water with UV detection at 254 nm and LSC analysis of the collected fractions. Column recoveries were 97.9-101.3%. Unextractable [^{14}C]residues remaining in the extracted soil were analyzed for total radioactivity by LSC following combustion. Detection limits were $\leq$0.01 ppm.

DATA SUMMARY:

Ring-labeled [^{14}C]pentachloronitrobenzene (PCNB, radiochemical purity 98.6%), at 10.467 ppm, dissipated with a registrant-calculated half-life of 77 days from sandy loam soil that was incubated in the dark at 25.3 $\pm$ 0.2°C. [^{14}C]PCNB declined from 94.9% of the applied immediately posttreatment to 50.1% at 91 days and to 3.1% at 365 days. The major degradate,

pentachloroaniline (PCA),

reached a maximum concentration of 12.9% of the applied at 122 days posttreatment. A second degradate

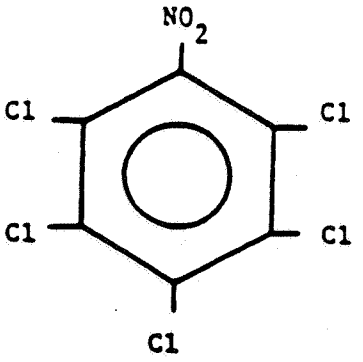
pentachlorothioanisole (PCTA),

reached a maximum of 1.9% of the applied at 30 days posttreatment. Polar compounds remaining at the TLC origin comprised up to 6.1% of

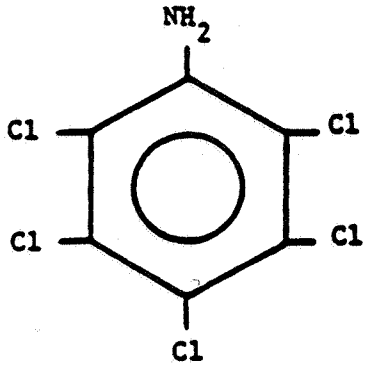
the applied. Unextractable PCNB residues were 7.4% at 273 days posttreatment and were 6.1% at 365 days posttreatment. At 365 days posttreatment, volatiles totaled 60.5% of the applied. Carbon dioxide totaled 0.4% of the applied, and other volatiles were

comprised of mostly PCNB and of smaller amounts of PCA. During the study, material balances ranged from 85.5 to 100% of the applied.

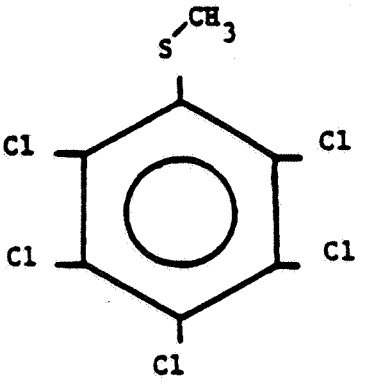
Chemical Structures of PCNB, PCA, PCTA, PCB and HCB



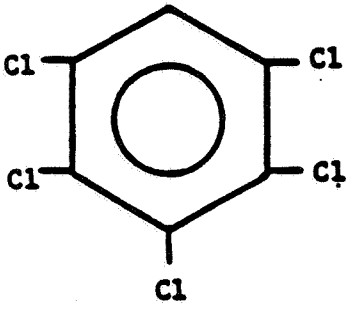
PCNB (Pentachloronitrobenzene)



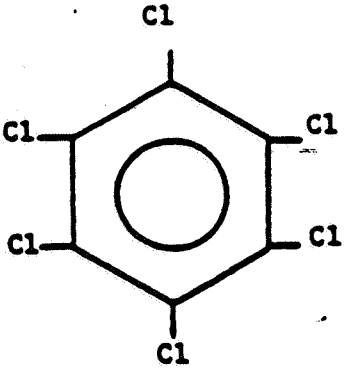
PCA (Pentachloroaniline)



PCTA (Pentachlorothioanisole)



PCB (Pentachlorobenzene)



HCB (Hexachlorobenzene)

PCNB environmental fate review

Page _____ is not included in this copy.

Pages 52 through 65 are not included in this copy.

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 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

X FIFRA registration data

___ The document is a duplicate of page(s) _____

___ The document is not responsive to the request

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.

DATA EVALUATION RECORD

STUDY 4

CHEM 056502 Pentachloronitrobenzene §162-2

FORMULATION--00--ACTIVE INGREDIENT

STUDY ID 41203602
Daly, D., and J. Schmidt. 1989. Anaerobic soil metabolism of ^{14}C-pentachloronitrobenzene. ABC Final Report No. 35905. Unpublished study performed by Analytical Bio-Chemistry Laboratories, Inc., Columbia, MO, and submitted by Uniroyal Chemical Company, Inc., Naugatuck, CT.

DIRECT REVIEW TIME = 15

REVIEWED BY: C. Little TITLE: Staff Scientist

EDITED BY: T. Colvin-Snyder TITLE: Staff Scientist
K. Patten Task Leader

APPROVED BY: W. Spangler TITLE: Project Manager

ORG: Dynamac Corporation
Rockville, MD

SECONDARY REVIEW BY: D. Spatz
TITLE: Chemist
ORG: EFGWB/EFED/OPP

SIGNATURE: DEC 28 1990

CONCLUSIONS:

Metabolism - Anaerobic Soil

1. This study cannot be used to fulfill the anaerobic soil metabolism data requirement.

2. Pentachloronitrobenzene (PCNB) dissipated under anaerobic conditions with an observed half-life of <30 days from sandy loam soil incubated in the dark at 25°C. Prior to establishing anaerobic conditions, the soil samples were incubated aerobically at a soil moisture of 75% of field capacity for 30 days. Nonvolatile degradates identified were pentachloroaniline (PCA), pentachlorothioanisole (PCTA), and pentachlorophenol (PCP). Volatilized residues included PCNB, PCA, PCTA, pentachlorobenzene (PCB), hexachlorobenzene (HCB), and carbon dioxide.

3. This study is unacceptable for the following reasons:

   a. Up to 17% of the [^{14}C]residues extracted from the soil (3 μg/g) and up to 67% of the residues in the flood water (0.4 μg/g) were not accounted for. The study authors did not specify whether these missing residues were unidentified degradates isolated on the TLC plates or were indistinguishable from background noise.

   b. The analytical methodology employed to separate and identify residues was insufficient. In this study, one-dimensional TLC with one solvent system was used to identify non-volatile residues and GC was employed to identify volatiles. Neither method provides confirmatory identification. Although GC-MS is preferred whenever feasible, HPLC and then 2-dimensional TLC may prove to be acceptable if the HPLC and TLC systems employ different mobile phases and the separations achieved are unequivocal.

   c. The soil extracts and flood water were stored frozen for an unspecified period of time prior to TLC analysis. Freezer storage stability data for PCNB and its degradates in soil extracts and flood water were not provided.

METHODOLOGY:

Uniformly ring-labeled pentachloronitrobenzene (radiochemical purity >98.9%, specific activity 8.9 mCi/mmol, Uniroyal), in acetonitrile, was added at a nominal rate of 25 ppm to 20 silanized culture tubes containing air-dried, sieved (2 mm) sandy loam soil (64% sand, 20% silt, 16% clay, pH 6.2, organic matter 1.6%, CEC 9.5 meq/100 g). An additional ten soil samples were prepared to serve as controls. The culture tubes containing treated soil were vortexed to ensure distribution of the pesticide, and deionized water was added to the soil samples to bring the moisture content to 75% of field capacity. The soil samples (treated and control) were placed in a 3000-mL resin pot which was connected, in series, to volatile traps of ethylene glycol, 1 N H_2SO_4 solution, and 1 N potassium hydroxide (two traps) (Figure 2). A rubber extension plug fitted into the center hole of the resin pot allowed for removal of the individual culture tubes. The soil samples were incubated aerobically in the dark at 25°C for 30 days. Following the aerobic incubation period, all of the soil samples were flooded with deionized water and the air flowing through the system was replaced with nitrogen in order to establish anaerobic conditions. Samples were collected for analysis at 0, 1, 3, 7, 14, and 30 days posttreatment during the aerobic incubation period, and at 60 and 90 days posttreatment during the anaerobic incubation period (30 and 60 days postflooding).

The water layer was removed from the flooded samples collected at 60 and 90 days posttreatment. Soil samples collected on days 0 and 1 were extracted three times by shaking with methanol; soil samples

collected at other intervals (including the soil fraction from the 60 and 90 day samples) were extracted four times by shaking with methanol:1 N acetic acid (80:20). The supernatant was removed by centrifugation, and triplicate aliquots of the soil extracts and the flood water were analyzed for total radioactivity by LSC. The soil extracts and flood water were stored frozen except during analysis. Triplicate subsamples of the extracted soil were analyzed by LSC following combustion.

The soil extracts and flood water were further analyzed using one-dimensional TLC on silica gel plates developed with hexane:toluene: acetone (7:3:1, v:v:v). The samples were cochromatographed with unlabeled reference standards. Radioactive zones on the plates were located and quantified using a radiochromatogram scanner; the zones were also visualized using autoradiography. Radioactive zones were identified by comparison with reference standards, which were visualized with UV light.

Each ethylene glycol trapping solution was partitioned three times with methylene chloride. Aliquots of the methylene chloride fraction were analyzed using LSC; the remaining methylene chloride was evaporated to dryness, and the resulting residues were redissolved in methanol and transferred into a tube. The residues were evaporated to dryness and reconstituted in methanol twice, then concentrated by partial evaporation. Aliquots of the concentrated methanol were analyzed by LSC and by GC with electron capture detection. Trapping solutions from the H_2SO_4 and potassium hydroxide volatile traps were analyzed for total radioactivity by LSC.

DATA SUMMARY:

Uniformly ring-labeled pentachloronitrobenzene (PCNB; radiochemical purity >98.9%) dissipated under anaerobic conditions (flooding plus nitrogen atmosphere) with an observed half-life of <30 days from sandy loam soil incubated in the dark at 25°C. PCNB declined from 9.65 µg/g immediately preflooding to 0.643 µg/g after 30 days of anaerobic incubation and 0.627 µg/g after 60 days. Prior to establishing anaerobic conditions, the soil samples were incubated aerobically for 30 days.

In the soil extracts, total PCNB residues were 17.7 µg/g immediately prior to flooding, and 15.9 and 16.5 µg/g after 30 and 60 days of anaerobic incubation, respectively; unextractable residues were 1.93, 2.44 and 2.02 µg/g at 0, 30, and 60 days postflooding, respectively. Degradates identified in the soil were

pentachloroaniline (PCA),

present at a maximum of 86.6% of the recovered from soil extracts at 30 days postflooding;

pentachlorothioanisole (PCTA),

present at a maximum of 3.2% of the recovered from soil extracts immediately preflooding; and

pentachlorophenol (PCP),

present at a maximum of 2.0% of the recovered from soil extracts at 60 days postflooding.

In the flood water, total PCNB residues recovered from the flood water were 0.563-0.643 μg/g; PCNB was 0.643 μg/g and 0.563 μg/g at 30 and 60 days postflooding, respectively. Degradates present in the water were PCA (25.2-28.3% of the radioactivity recovered in the flood water) and PCP (6.6-7.5% of the radioactivity recovered in the flood water).

Volatiles totaled 1.25 μg/g immediately prior to establishment of anaerobic conditions and 2.24 μg/g at 60 days postflooding. Volatiles were mostly of PCNB and PCA, and smaller amounts of carbon dioxide; small amounts of pentachlorobenzene (PCB) and hexachlorobenzene (HCB) were isolated only immediately prior to flooding.

During the study, material balances ranged from 96.0 to 100% of the applied radioactivity.

COMMENTS:

1. The study authors calculated a dissipation half-life of PCNB from soil of 15.4 days; however, since this half-life was calculated solely from three data points (0, 30 and 60 days after anaerobic conditions were established), the accuracy of this estimate is questionable. Therefore, the observed half-life of <30 days was reported in this review.

2. Fortified soil was used to determine parent compound recoveries for LSC following combustion; the reported concentrations of unextractable radioactivity were corrected for recovery efficiencies.

DATA EVALUATION RECORD

STUDY 5

CHEM 056502 Pentachloronitrobenzene (PCNB) §163-2

FORMULATION--06--WETTABLE POWDER (WP)

STUDY ID 40580201
Teeter, D. 1988. Laboratory volatility from soil of PCNB. Laboratory Project ID ABC #36283. Unpublished study performed by Analytical Bio-Chemistry Laboratories, Columbia, MO, and submitted by Uniroyal Chemical Company, Middlebury, CT.

DIRECT REVIEW TIME = 12

REVIEWED BY: N. Glassbrook TITLE: Staff Scientist

EDITED BY: T. Colvin-Snyder TITLE: Staff Scientist
K. Patten Task Leader

APPROVED BY: W. Spangler TITLE: Project Manager

ORG: Dynamac Corporation
Rockville, MD

SECONDARY REVIEW BY: D. Spatz
TITLE: Chemist
ORG: EFGWB/EFED/OPP

SIGNATURE: DEC 28 1990

CONCLUSIONS:

Mobility - Laboratory Volatility

1. This study cannot be used to fulfill the Laboratory Volatility data requirement.

2. This study is unacceptable for the following reasons:

   a. The soil was not analyzed for PCNB residues; therefore, the application rate was not verified and material balances were not determined.

   b. The soil was autoclaved before the test. Autoclaving of soils may significantly change the physical and chemical properties of the soils which may affect the adsorption of pesticides by the soils. Autoclaving may cause the soil to become more hydrophobic, or the soil CEC may change as a result of the breakdown of organic matter and/or the expansion of the

crystalline structure of the clay particles. How autoclaving affected PCNB volatilization from this soil is unknown.

METHODOLOGY:

Pentachloronitrobenzene (PCNB,; Terraclor 75W, 75% WP, source unspecified) was incorporated into subsamples of sieved (2 mm) autoclaved sandy loam soil (64% sand, 20% silt, 16% clay, 1.6% organic matter, pH 6.2, CEC 9.5 meq/100 g) at 38-43 ppm. The soil samples were placed in glass containers with screw caps and allowed to sit overnight. The soil samples were then placed in test chambers and incubated at 25 ± 1°C and 25, 50, or 75% of field capacity. Humidified air (flow rate varying between 71 and 281 mL/min) was drawn continuously though each chamber and then through two polyurethane foam plugs which served as traps for volatilized PCNB (Figure 1). Foam plugs were removed for analysis at four intervals up to 9940-11080 minutes posttreatment (6.9-7.7 days).

The foam plugs were extracted four times with hexane, and the total volume of the combined extracts was adjusted with iso-octane. The quantity of PCNB in the extracts was determined by GC with a silicone stationary phase on a diatomaceous support, nitrogen as a carrier gas, and an electron capture detector.

Vapor trapping efficiencies for the foam plugs were tested in a preliminary experiment by applying PCNB to foam plugs and passing air through them at 250 mL/min for 1 to 4 days. Recovery efficiencies ranged from 84.4 to 121% of the applied.

DATA SUMMARY:

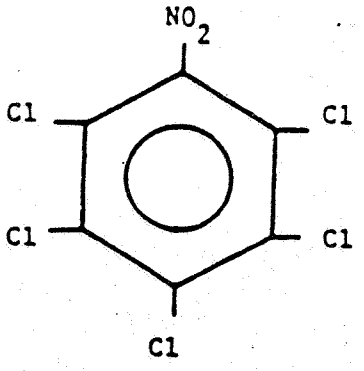
Less than 1% of the pentachloronitrobenzene (PCNB, 75% WP) applied to moist (25, 50, or 75% of field capacity) sterile sandy loam soil at a nominal concentration of 43 ppm was volatilized from the soil during 6.9 to 7.7 days of incubation in the dark at 25 ± 1°C. During the study, air flow through the experimental system varied between 71 and 281 mL/min.

The calculated vapor pressure of PCNB varied from 4.2×10^{-6} to 5.7×10^{-5} mm Hg, the volatility ranged from 4.9×10^{-4} to 1.5×10^{-2} $\mu g/cm^2 \cdot hr$, and the vapor density ranged from 77 to 200 $\mu g/m^3$.

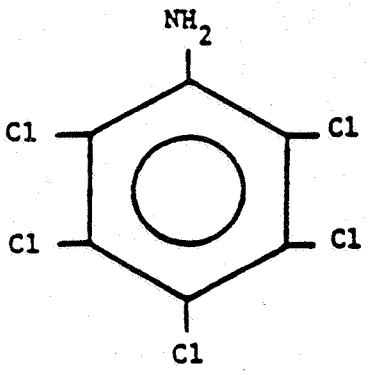
COMMENTS:

1. The pH of the sandy loam soil was not listed in Table 1 of this study. The value reported by the reviewer was obtained from Table 1 of "Aerobic soil metabolism of ^{14}C-pentachloronitrobenzene", ABC #35904 (MRID 41203601) in which the same blue sandy loam soil was used.

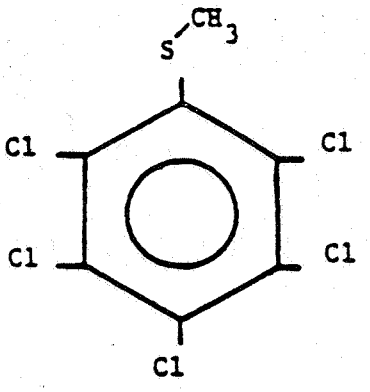
Chemical Structures of PCNB, PCA, PCTA, PCB and HCB



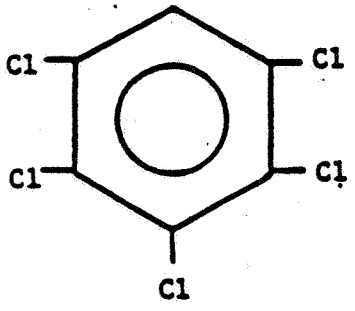
PCNB (Pentachloronitrobenzene)



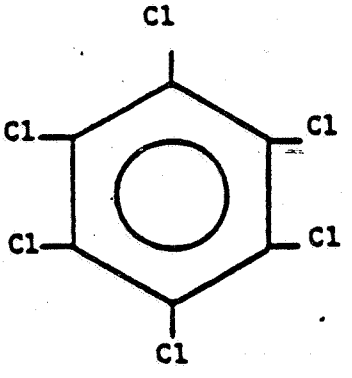
PCA (Pentachloroaniline)



PCTA (Pentachlorothioanisole)



PCB (Pentachlorobenzene)



HCB (Hexachlorobenzene)

PCNB environmental fate review

Page _____ is not included in this copy.

Pages 87 through 88 are not included in this copy.

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 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

X FIFRA registration data

___ The document is a duplicate of page(s) _____

___ The document is not responsive to the request

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.

DATA EVALUATION RECORD

STUDY 6

CHEM 056502 Pentachloronitrobenzene (PCNB) §163-2

FORMULATION--12--EMULSIFIABLE CONCENTRATE

STUDY ID 41178001
Bowman, B.R. 1988. Laboratory volatility from soil of PCNB. ABC Final Report No. 37090. Unpublished study performed by Analytical Bio-Chemistry Laboratories, Columbia, MO, and submitted by AMVAC Chemical Corporation, Los Angeles, CA.

DIRECT REVIEW TIME = 12

REVIEWED BY: N. Glassbrook TITLE: Staff Scientist

EDITED BY: T. Colvin-Snyder TITLE: Staff Scientist
K. Patten Task Leader

APPROVED BY: W. Spangler TITLE: Project Manager

ORG: Dynamac Corporation
Rockville, MD

SECONDARY REVIEW BY: D. Spatz
TITLE: Chemist
ORG: EFGWB/EFED/OPP

SIGNATURE: DEC 28 1990

CONCLUSIONS:

Mobility - Laboratory Volatility

1. This study can be used to fulfill the Laboratory Volatility data requirement.

2. The volatility of pentachloronitrobenzene (PCNB) from sandy loam soil incubated in the dark at 50 or 75% of field moisture capacity and 25°C, ranged from 0.0622 to 0.171 $\mu g/cm^2/hr$. The calculated vapor pressure ranged from 3.14×10^{-5} mmHg to 8.19×10^{-5} mmHg and the vapor density ranged from 4.99×10^{-4} to 1.30×10^{-3} g/m^3. At 7 days posttreatment, volatilized PCNB residues totaled 1556-1650 μg (approximately 80% of the applied). Air flow through the system was 283-311 mL/min. PCNB was the only volatile residue found. During the study, material balances ranged from 90.3 to 111% of the applied.

3. This study is acceptable and fulfills EPA Data Requirements for Registering Pesticides by providing information on the volatility of pentachloronitrobenzene under laboratory conditions.

METHODOLOGY:

A mixture of formulated pentachloronitrobenzene (PCNB; 2E, 24% PCNB, source unspecified) plus uniformly ring-labeled [^{14}C]PCNB (radiochemical purity >98%, specific activity 46.4 mCi/mmol, source unspecified) dissolved in hexane (specific activity of mixture 4084 dpm/μg) was incorporated into sieved (2 mm) sandy loam soil (64% sand, 20% silt, 16% clay, 1.6% organic matter, pH 6.2, CEC 9.5 meq/100 g) in glass petri dishes at a nominal concentration of 20 ppm. The moisture content of the soil had been adjusted to 50 or 75% of field capacity prior to the addition of the PCNB. Two petri dishes of soil were then sealed inside each of eleven chambers constructed from cake pans lined with non-stick enamel. Humidified air was continuously drawn at 283-311 mL/min through each chamber, then through two polyurethane foam plugs which served as traps for volatilized PCNB. Soil, foam plugs, and the test chambers were removed for analysis at 15 hours, 1 day, 3 days, 5 days, and 7 days posttreatment.

The foam plugs were extracted four times with hexane. The chambers and the bottles which contained the foam plugs were rinsed with methanol. The silicone rubber tubing used to seal the chambers of day 5 and 7 samples was cut up and extracted with methanol. The hexane and methanol extracts were analyzed by LSC for total radioactivity and by TLC for PCNB, manufacturing by-products, and degradates. Silica gel TLC plates containing a fluorescent indicator were developed in hexane. Nonradiolabeled reference standards of PCNB, pentachlorobenzene (PCB), hexachlorobenzene (HCB), pentachloroanailine (PCA), and pentachlorothioanaisole (PCTA) were cochromatographed with the extracts. Radioactive areas on the TLC plates were located and quantified with a TLC scanner and identified by comparison to the nonlabeled standards, which were located using UV light. In addition, extracts from day 7 samples were analyzed by GC. The GC analysis was conducted using an unspecified column, helium as the carrier gas, and electron capture detection.

Soil samples were extracted twice with methanol:1 N acetic acid (80:20) and once with acetone; the composite extracts were analyzed by LSC for total radioactivity. Following extraction, the remaining soil was analyzed for total radioactivity by LSC following combustion.

COMMENTS:

1. The application rate was verified by direct analysis of the treatment solution rather than analysis of the soil immediately posttreatment. The reported material balances are based on the amount of radioactivity present in the treatment solution.

2. Vapor trapping efficiencies for the foam plugs were tested in a preliminary experiment by applying PCNB directly to the foam plugs, passing air through the treated plugs for 4 days, and finally extracting the plugs with hexane. Recoveries from foam plugs extracted as in the definitive study were ≥97.7%.

3. Due to a low material balance for one replicate of the day 5 sample at 75% of field capacity, the results of this replicate were rejected and the test was repeated. The results of the repeat experiment are designated D5R-75% in the data tables.

4. The soil extraction procedure in the methods section states that the soil was extracted three times with methanol:acetic acid (80:20); however, the laboratory note on soil extraction in the Appendix (p. 152) gives the extraction procedure as twice with methanol:acetic acid and once with acetone.

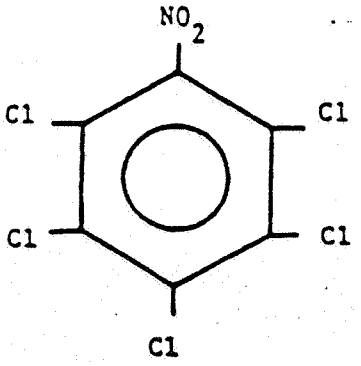
5. The silicone rubber tubing used to seal the incubation chambers adsorbed some volatiles (30.2% of the total volatiles by day 7 at 75% field capacity). Analysis of the residues extracted from the tubing used to seal chambers for day 5 and 7 samples indicated that there was unidentified labeled material present in the tubing extracts that was not present in the rinse from the cake pans or in the polyurethane traps. This unidentified material remained at the origin of TLC plates and comprised 11-16% of the radioactivity recovered from the tubing (<5% of the applied).

6. The values reported for volatiles are the sums of residues recovered from the foam plugs, pan rinsate, and tubing extracts.

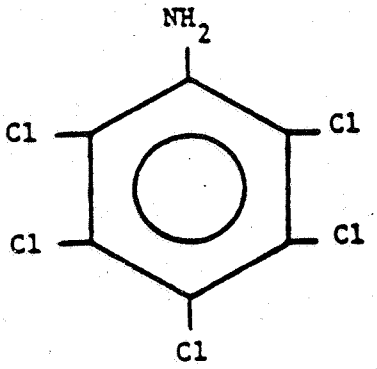
7. A batch equilibrium study was performed to determine the soil adsorption coefficient of PCNB in sandy loam soil. Since the soil was autoclaved for the batch equilibrium experiment, but was not autoclaved for the volatility experiment, the value of the results of this study in predicting the mobility of PCNB in the test soil under the conditions used in this volatility study is questionable. Autoclaving of soils may significantly change the physical and chemical properties of the soils which may affect the adsorption of pesticides by the soils. Autoclaving may cause the soil to become more hydrophobic, or the soil CEC may change as a result of the breakdown of organic matter and/or the expansion of the crystalline structure of the clay particles.

   Based on the results of this experiment, PCNB was determined to be mobile in autoclaved sandy loam soil; the Freundlich K_{ads} was 31.4.

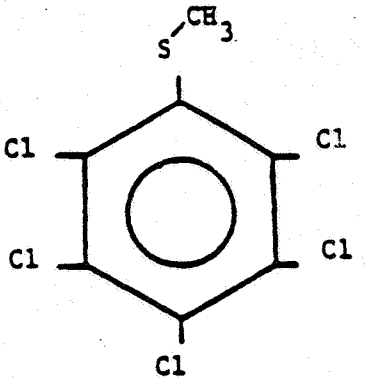
Chemical Structures of PCNB, PCA, PCTA, PCB and HCB



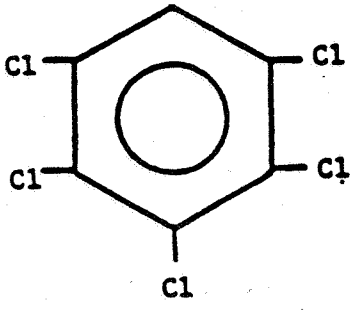
PCNB (Pentachloronitrobenzene)



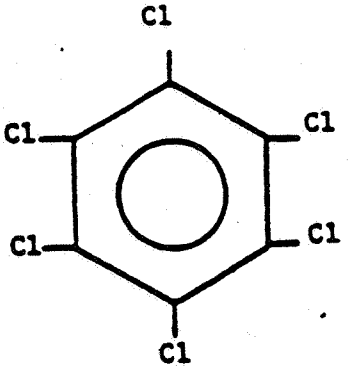
PCA (Pentachloroaniline)



PCTA (Pentachlorothioanisole)



PCB (Pentachlorobenzene)



HCB (Hexachlorobenzene)

PCNB environmental fate review

Page _____ is not included in this copy.

Pages 93 through 97 are not included in this copy.

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 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

X FIFRA registration data

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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.

DATA EVALUATION RECORD

STUDY 7

CHEM 056502 **Pentachloronitrobenzene** §164-1

FORMULATION--06--WETTABLE POWDER (WP)

STUDY ID 41210501
Irissarri, G. and M. Lengen. 1989. Field dissipation of pentachloronitrobenzene on a California turf site. Uniroyal Project No. 8785. Unpublished study performed by California Agricultural Research, Inc., Kerman, CA; North Coast Laboratories, Inc., Arcata, CA; and Uniroyal Chemical Co., Inc., Middlebury, CT; and submitted by Uniroyal Chemical Co., Inc., Middlebury, CT.

DIRECT RVW TIME = 6

REVIEWED BY: L. Binari TITLE: Staff Scientist

EDITED BY: T. Colvin-Snyder TITLE: Staff Scientist
K. Patten Task Leader

APPROVED BY: W. Spangler TITLE: Project Manager

ORG: Dynamac Corporation
Rockville, MD

SECONDARY REVIEW BY: D. Spatz
TITLE: Chemist
ORG: EFGWB/EFED/OPP

SIGNATURE: DEC 28 1990

CONCLUSIONS:

Field Dissipation - Terrestrial

1. This study cannot be used to fulfill the Soil Field Dissipation data requirement.

2. This study is unacceptable for the following reasons:

   a. The declared application rate (32.7 lb ai/A) was not confirmed by the soil samples taken immediately posttreatment or 1 day posttreatment. An application rate of 32.7 lb ai/A is equivalent to approximately 16 ppm in a 6-inch soil core. However, residues in the 0-6 inch soil sample measured only 6.2 ppm immediately posttreatment and 8.5 ppm 1-day posttreatment. No explanation was given for this discrepancy.

b. The grass was mowed 2 days after the first application. Since an unknown amount of PCNB would still be on the grass clippings and these clippings were either bagged or possibly blown off site (not specified in the report), the data cannot be used to accurately assess the dissipation of PCNB. This mowing may also explain the significant decrease in measured residues found on day 3 posttreatment as compared to those recorded on day 1 (3.6 ppm and 8.5 ppm, respectively).

c. Only 3 soil cores were sampled per sampling interval. This degree of replication is insufficient. A minimum of 15 soil cores with a minimum of three composites must be taken per sampling interval at each plot.

d. Residues were identified using only gas chromatography. This approach does not give confirmatory identification. Although GC-MS is preferred whenever feasible, GC or HPLC and then 2-dimensional TLC may prove to be acceptable if the HPLC and TLC systems employ different mobile phases and the separations achieved are unequivocal.

e. The registrant-calculated half-life of 35 days was determined based upon the second application being day 0. However, the sampling intervals were inadequate to define this half-life. The soil was not sampled until 32 days after the second treatment.

f. Daily rainfall and air temperature data were not provided, only monthly summaries. Soil temperature data were not provided.

g. Although frozen storage stability data were provided by the registrant, the study authors did not report how long the soil samples were stored frozen prior to analysis; therefore, the results of this field dissipation experiment could not be integrated with the available stability data.

h. Data from the control plot were not provided.

3. PCNB dissipated with a half-life of 35 days from the upper 6 inches of a Bermuda grass turf plot of sandy loam soil in California following the second of two treatments (33-day interval) of PCNB (Terraclor, 75% WP) at 1.0 lb of formulation/1000 feet^2/treatment (32.7 lb ai/A; which is the maximum label rate). The degradates pentachloroaniline, pentachlorothioanisole, and pentachlorobenzene were detected in the 0- to 6-inch soil layer up to 360 days posttreatment. Hexachlorobenzene was detected in the 0- to 6- inch soil layer up to 179 days posttreatment. PCNB and its degradates did not appear to leach below the 6-inch depth.

METHODOLOGY:

PCNB (Terraclor, 75% WP, Uniroyal Chemical) was applied twice, at 32.7 lb ai/A/application (1.0 lb of formulation/1000 feet^2/ application; the maximum label rate), to a bermudagrass turf plot (50 x 50 feet) of sandy loam soil (69% sand, 21% silt, 10% clay, 0.66% organic matter, pH 6.1, CEC 4.1 meq/100 g) located near Kerman, California, on November 9 and December 7, 1987. Following each application, the plot was irrigated by sprinkler. An untreated plot (size unspecified) located 229 feet north of the treated plot was maintained as a control. The plots were periodically mowed during the study. Soil samples were taken in 6-inch increments to a maximum depth of 5 feet prior to each treatment, at intervals between 0 and 28 days after the first treatment, and at intervals between 0 and 332 days after the second treatment. Soil samples were collected from the 0- to 6-inch depth using a soil probe (diameter unspecified). In order to sample depths below 6 inches, the surface 6 inches of soil were removed. A guard sleeve was placed around the sampling hole, and a bucket auger (2 3/4-inch diameter) was inserted into the soil to a depth of 6 inches. The top 1 inch of soil within the auger was discarded, then two samples were collected from the soil remaining within the auger and combined. The procedure was repeated for each 6-inch increment to a depth of 24 inches. Three soil subsamples were collected from the treated plot at each sampling interval. Soil samples were stored frozen for an unspecified period of time prior to extraction.

Soil samples (25 g) were extracted with acetone. The acetone extract was combined with water, then partitioned twice with hexane. The hexane phases were filtered through sodium sulfate, combined, and concentrated, then analyzed for PCNB and its degradates using GC with electron capture detection. The detection limit was 0.005 ppm. Mean recovery efficiencies from soil samples fortified with PCNB and its degradates at unspecified concentrations were 97.0% of the applied for PCNB, 98.3% for pentachloroaniline, 99.7% for pentachlorothioanisole, 94.7% for pentachlorobenzene, and 95.2% for hexachlorobenzene.

DATA SUMMARY:

Pentachloronitrobenzene (PCNB) dissipated with a registrant-calculated half-life of 35 days from the upper 6 inches of a Bermuda grass turf plot (50 x 50 feet) of sandy loam soil in California following the second of two applications (33-day interval) of PCNB (Terraclor, 75% WP) at 32.7 lb ai/A/application (1.0 lb of formulation/1000 feet^2/application). In the 0- to 6-inch soil depth after the second application of PCNB, PCNB decreased from 8.60 ppm immediately posttreatment to 3.433 ppm at 63 days, 1.40 ppm at 122 days, and 0.0127 ppm at 332 days. Maximum concentrations of PCNB degradates in the 0- to 6-inch soil depth were 0.430 ppm for pentachloroaniline (PCA) at 242 days after the second treatment,

0.117 ppm for pentachlorothioanisole (PCTA) at 242 days after the second treatment, 0.031 ppm for pentachlorobenzene (PCB) at 151 days after the second treatment, and 0.076 ppm for hexachlorobenzene (HCB) immediately following the second treatment. In the 6- to 12-inch soil depth, PCNB was detected at 0.028 and 0.011 ppm at 0 and 1 day after the first treatment, respectively, and 0.007 ppm immediately after the second treatment only. PCNB was not detected (<0.005 ppm) in the 12- to 18-inch soil layer and was detected once, at 0.967 ppm at 5 days after the first treatment, in the 18- to 24-inch depth. In general, PCNB degradates were <0.01 ppm in the 6- to 12-, 12- to 18-, and 18- to 24-inch depths.

From November 1987 to November 1988, rainfall plus irrigation totaled 32.78 inches and air temperatures ranged from 20 to 107°F. The depth to the water table was 80 feet, and the slope of the field was 1%.

COMMENTS:

1. In the storage stability experiment, soil was treated with PCNB (0.1 and 5.0 ppm) or its degradates (0.1 ppm) and stored frozen for up to 6 months. In soil fortified with PCNB at 5.0 ppm, 78-104% of the applied was recovered after 1-6 months of storage. In soil fortified with PCNB, PCB, and HCB at 0.1 ppm, recoveries ranged from approximately 88 to 94% of the applied after 1 month of storage, then decreased to approximately 74 to 87% after 2-6 months. In soil fortified with PCA and PCTA at 0.1 ppm, recoveries ranged from 106 to 132% and 89 to 115%, respectively, after 1-6 months of storage.

2. The pattern of decline of PCNB in the 0- to 6-inch soil layer after the first treatment and prior to the second treatment was variable, but following the second treatment PCNB declined steadily.

3. It was reported that soil samples were also to be collected 512 days after the second treatment (May 1, 1989), but results from analysis of those samples were not provided.

4. The study author suggested that the isolated incidents of residues detected below the 0- to 6-inch soil layer were the result of contamination rather than leaching.

5. The treated plot received one application of ammonium sulfate (20 lb/plot) on October 12, 1987, and one application of "Green Sweep" (1 quart/plot) on March 16, 1988.

PCNB environmental fate review

Page 102 is not included in this copy.

Pages _____ through _____ are not included in this copy.

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 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

X FIFRA registration data

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PCNB environmental fate review

Page _____ is not included in this copy.

Pages 71 through 83 are not included in this copy.

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 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

X FIFRA registration data

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DATA EVALUATION RECORD

STUDY 8

CHEM 056502 Pentachloronitrobenzene §164-1

FORMULATION--06--WETTABLE POWDER (WP)

STUDY ID 41216401
Rice, F., B. Jacobson, and M.W. Winberry. 1989. Terrestrial field dissipation for PCNB in broccoli. Uniroyal Project No. 8754B. Unpublished study performed by Pan Agricultural Laboratories, Madera, CA and Analytical Bio-Chemistry Laboratories, Inc., Columbia, MO; and submitted by Uniroyal Chemical Co., Inc., Middlebury, CT.

DIRECT RVW TIME = 6

REVIEWED BY: L. Binari TITLE: Staff Scientist

EDITED BY: N. Glassbrook TITLE: Staff Scientist
T. Colvin-Snyder Staff Scientist

APPROVED BY: W. Spangler TITLE: Project Manager

ORG: Dynamac Corporation
Rockville, MD

SECONDARY REVIEW BY: D. Spatz
TITLE: Chemist
ORG: EFGWB/EFED/OPP

SIGNATURE: DEC 28 1990

CONCLUSIONS:

Field Dissipation - Terrestrial

1. This study cannot be used to fulfill the Soil Field Dissipation data requirement.

2. This study is unacceptable for the following reasons:

   a. The submitted freezer storage stability data indicate that many of the test samples were stored for longer than what the stability data permits before significant degradation takes place. The storage stability data supports a 120-day storage interval for PCNB, but only a 30-day interval for the metabolite PCB and the contaminant HCB. After this period of time, significant degradation was apparent. Many field test samples were stored for a period in excess of 120 days. The result of this excessive storage interval surely compromised the validity of the study.

b. The application rate was not confirmed by the immediately post-application residue measurement. At an application rate of 30 lbs ai/acre, there should have been ≈15.0 ppm in the soil (6-inch depth). However, the post-application sampling interval showed only 4.7 ppm and day 1 posttreatment measured only 7.7 ppm (the maximum level found throughout the study). The authors suggest that the volatility of PCNB may explain this loss, however, considering that the product was incorporated 4-6 inches into the soil immediately after treatment, their suggestion does not seem to account for a loss of ≈50% of the applied PCNB.

c. Residues were identified using only gas chromatography. This approach does not give confirmatory identification. Although GC-MS is preferred whenever feasible, GC or HPLC and then 2-dimensional TLC may prove to be acceptable if the HPLC and TLC systems employ different mobile phases and the separations achieved are unequivocal.

METHODOLOGY:

PCNB (Terraclor, 75% WP) was applied at 30 lb ai/A (maximum label rate) as a preplant broadcast spray to a field plot (33.3 x 100 feet) of loamy sand soil (0- to 12-inch layer; 79% sand, 13% silt, 8% clay, 0.4% organic matter, pH 5.6, CEC 4.4 meq/100 g) located near Madera, California, on September 24, 1987. Immediately posttreatment, the soil was cultivated to a depth of 4-6 inches and planted to broccoli. An untreated plot (same size) also planted to broccoli was maintained as a control. During the study, the plots were periodically hand cultivated. Fifteen soil cores (1-inch diameter x 24-inch depth) were taken prior to treatment and at intervals between 0 and 543 days posttreatment.

Prior to analysis, soil cores were divided into 0- to 6-, 6- to 12-, 12-to 18-, and 18- to 24-inch segments. Samples of similar depth were combined to yield three composite samples for each depth at each interval. Each composite sample was homogenized, and a subsample (50 g) was extracted with acetone. The acetone extract was filtered, combined with water and salt, then partitioned twice with hexane. Hexane phases were filtered through anhydrous sodium sulfate. The combined hexane extract was reduced to dryness, redissolved in 2,2,4-trimethylpentane, and then analyzed for PCNB and its degradates using GC with electron capture detection. The detection limit was 0.005 ppm. Recovery efficiencies from soil samples fortified at 0.005-5.0 ppm ranged from 63 to 118% of the applied for PCNB, 77 to 112% for pentachloroaniline, 34 to 118% for pentachlorothioanisole, 0 to 110% for pentachlorobenzene, and 48 to 120% for hexachlorobenzene. Residue concentrations in the soil were corrected for method recoveries.

DATA SUMMARY:

Pentachloronitrobenzene (PCNB) dissipated with a registrant-calculated half-life of 128 days from the upper 6 inches of a field plot (33.3 x 100 feet) of loamy sand soil in California treated with PCNB (Terraclor, 75% WP) at 30 lb ai/A on September 24, 1987. In the 0- to 6-inch soil depth, the average PCNB concentration was 4.3 ppm immediately posttreatment, increased to 6.9 ppm (maximum 9.9 ppm) at 1 day posttreatment, decreased to 2.7 ppm at 28 days, ranged from 1.9 to 3.8 ppm between 56 and 126 days, and declined to 0.30 ppm at 543 days. In the 0- to 6-inch soil depth, the degradate pentachlorobenzene (PCB) reached an average maximum concentration of 0.20 ppm at 56 days posttreatment; pentachlorothioanisole (PCTA) was a maximum of 0.40 ppm at 28 days; pentachloroaniline (PCA) was a maximum of 0.94 ppm at 455 days; and hexachlorobenzene (HCB) was a maximum of 0.056 ppm at 543 days. At lower soil depths, PCNB was detected in the 6- to 12-inch soil layer at 0.0063 ppm immediately posttreatment, 0.0058 ppm at 7 days, and 0.0056 ppm at 126 days; PCNB was not detected (<0.005 ppm) at other sampling intervals. In the 12-to 18-inch soil layer, PCNB was not detected; however, in the 18- to 24-inch soil layer, PCNB was detected at two sampling intervals (0.0083 ppm at 7 days posttreatment and 0.056 ppm at 182 days). In the 6- to 12-inch soil layer, the degradate PCB increased to 0.015 ppm by 543 days posttreatment; PCTA, PCA, and HCB were not detected (<0.005 ppm). PCNB degradates were not detected in the 12- to 18-inch soil layer. In the 18-to 24-inch soil layer, PCA and PCTA were detected at one sampling interval (182 days posttreatment) at 0.023 and 0.0084 ppm, respectively; PCB and HCB were not detected at this depth.

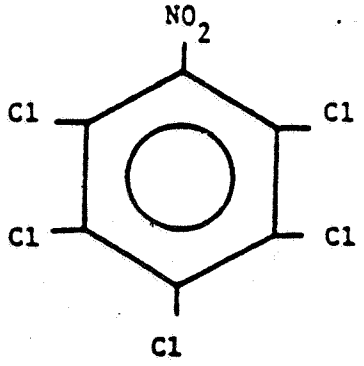
During the study, rainfall plus irrigation totaled 41.73 inches, air temperatures ranged from 24 to 105°F, and soil temperatures (8-inch depth) ranged from 33 to 104°F. The depth to the water table was approximately 95 feet, and the slope of the field was <1%.

COMMENTS:

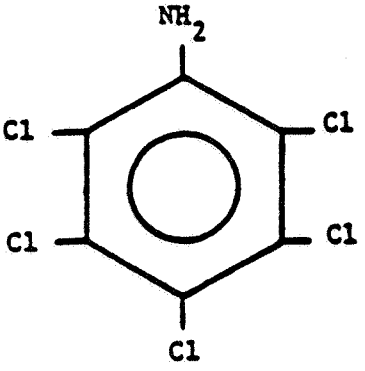
1. The study author stated that the isolated incidents of residues detected below the 0- to 6-inch soil layer were believed to be the result of contamination rather than leaching. This appears to be the case for the isolated detections of PCNB, PCA, and PCTA; however, the data indicate that PCB did leach into the 6- to 12-inch soil layer. PCB, which increased to 0.015 ppm by 543 days posttreatment, was detected in all three composite soil samples at 364, 455, and 543 days posttreatment and appeared to be following a normal leaching pattern.

2. The plots received trifluralin to remove weeds, but the number of applications and dates were not provided.

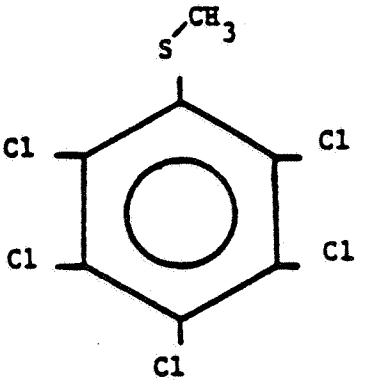
Chemical Structures of PCNB, PCA, PCTA, PCB and HCB



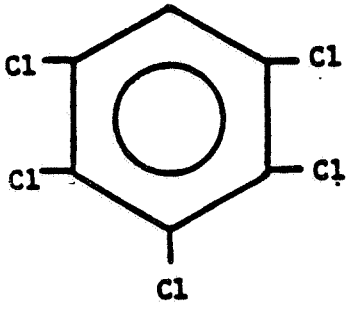
PCNB (Pentachloronitrobenzene)



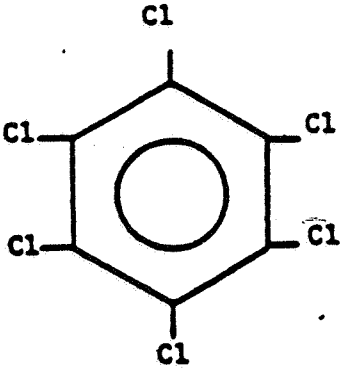
PCA (Pentachloroaniline)



PCTA (Pentachlorothioanisole)



PCB (Pentachlorobenzene)



HCB (Hexachlorobenzene)

PCNB environmental fate review

Page _____ is not included in this copy.

Pages 107 through 120 are not included in this copy.

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 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

X FIFRA registration data

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DATA EVALUATION RECORD

STUDY 9

CHEM 056502 Pentachloronitrobenzene §164-1

FORMULATION--12--EMULSIFIABLE CONCENTRATE (EC)

STUDY ID 41216402
Rice, F., B. Jacobson, and M.W. Winberry. 1989. Terrestrial field dissipation for PCNB in potatoes. Uniroyal Project No. 8754C. Unpublished study performed by Agricultural Division Hill Hall of University of Minnesota, Crookston, MN, and Analytical Bio-Chemistry Laboratories, Inc., Columbia, MO; and submitted by Uniroyal Chemical Co., Inc., Middlebury, CT.

DIRECT RVW TIME = 4

REVIEWED BY: L. Binari TITLE: Staff Scientist

EDITED BY: N. Glassbrook TITLE: Staff Scientist
T. Colvin-Snyder Staff Scientist

APPROVED BY: W. Spangler TITLE: Project Manager

ORG: Dynamac Corporation
Rockville, MD

SECONDARY REVIEW BY: D. Spatz
TITLE: Chemist
ORG: EFGWB/EFED/OPP
SIGNATURE:

DEC 28 1990

CONCLUSIONS:

Field Dissipation - Terrestrial

1. This study cannot be used to fulfill the Soil Field Dissipation data requirement.

2. This study is unacceptable for the following reasons:

   a. The application rate was not confirmed by the immediately post-application residue measurement. At an application rate of 25 lbs ai/acre, there should have been ≈12.5 ppm in the soil (6-inch depth). However, the post-application sampling interval showed only 4.2 ppm. The authors suggest that the volatility of PCNB may explain this loss, however, considering that the product was incorporated 4-6 inches into the soil immediately after treatment, their suggestion does not seem to account for a loss of >50% of the applied PCNB.

b. Residues were identified using only gas chromatography. This approach does not give confirmatory identification. Although GC-MS is preferred whenever feasible, GC or HPLC and then 2-dimensional TLC may prove to be acceptable if the HPLC and TLC systems employ different mobile phases and the separations achieved are unequivocal.

c. The submitted freezer storage stability data indicate that many of the test samples were stored for longer than what the stability data permits before significant degradation takes place. The storage stability data supports a 45-day storage interval for PCB. After this period of time, significant degradation was apparent. Many field test samples were stored for a period in excess of 60 days. The result of this storage interval surely compromised the validity of the study. In addition, the freezer storage stability data for HCB was highly variable and greater than 100% for eight of the thirteen sampling days (67-144%).

d. The variability in the data was such that the dissipation of PCNB could not be adequately explained using first-order kinetics. The r^2 value for the dissipation of PCNB in the 0-6" layer using first-order kinetics was a poor 0.83.

METHODOLOGY:

Pentachloronitrobenzene (PCNB, Terraclor, 2 lb/gallon EC) was applied at 25 lb ai/A as a preplant broadcast spray to a field plot (35 x 100 feet) of sandy loam soil (0- to 12-inch layer; 66% sand, 22% silt, 12% clay, 4.3% organic matter, pH 8.1, CEC 15.5 meq/100 g) located near Crookston, Minnesota, on June 19, 1987. Immediately posttreatment, the soil was cultivated to a depth of 4-6 inches and planted to potatoes. An untreated plot of the same size also planted to potatoes was maintained as a control. During the study, the plots were periodically hand cultivated. Fifteen soil cores (1-inch diameter, 24-inch depth) were taken prior to treatment and at intervals between 0 and 546 days posttreatment. Soil samples from the treated plot were stored frozen for approximately 21-221 days until processed for extraction.

Prior to analysis, soil cores were divided into 0- to 6-, 6- to 12-, 12-to 18-, and 18- to 24-inch segments. Samples of similar depth were combined to yield three composite samples for each depth at each interval. Each composite sample was homogenized, and a subsample (50 g) was extracted with acetone. The acetone extract was filtered, combined with water and salt, then partitioned twice with hexane. Hexane phases were filtered through anhydrous sodium sulfate. The combined hexane extract was reduced to dryness, redissolved in 2,2,4-trimethylpentane, and then analyzed for PCNB and its degradates using GC with electron-capture detection. The detection limit was 0.005 ppm. Recovery efficiencies from soil samples fortified at 0.005-5.0

ppm ranged from 76 to 136% of the applied for PCNB, 60 to 124% for pentachloroaniline, 74 to 141% for pentachlorothioanisole, 10 to 168% for pentachlorobenzene, and 40 to 150% for hexachlorobenzene. Residue concentrations in the soil were corrected for method recoveries.

DATA SUMMARY:

Pentachloronitrobenzene (PCNB) dissipated with a registrant-calculated half-life of 193 days from the upper 6 inches of a field plot (35 x 100 feet) of sandy loam soil in Minnesota treated with PCNB (Terraclor, 2 lb/gallon EC) at 25 lb ai/A on June 19, 1987. In the 0- to 6-inch soil depth, the average PCNB concentration was 4.1 ppm immediately posttreatment, was 3.2 ppm at 7 days, increased to 5.8 ppm at 14 days, decreased to 2.0 ppm by 298 days, and was 0.67 ppm at 546 days. In the 0- to 6-inch soil depth, the degradates pentachloroaniline (PCA) and pentachlorobenzene (PCB) gradually reached maximum concentrations of 1.1 and 0.18 ppm, respectively, by 546 days posttreatment. Pentachlorothioanisole (PCTA) was a maximum of 0.12 ppm at 56 days; and hexachlorobenzene (HCB) was a maximum of 0.025 ppm at 56-84 days. At lower soil depths, PCNB was detected in the 6- to 12-inch soil layer at 0.010-0.011 ppm at 1-14 days posttreatment and at 0.0077 ppm at 126 days; PCNB was not detected (<0.005 ppm) at other sampling intervals. In the 12- to 18-inch soil layer, PCNB was 0.0067 ppm immediately posttreatment, 0.032 ppm at 28 days, and 0.009 ppm at 56 days; and in the 18- to 24-inch soil layer, PCNB was at 0.0076-0.021 ppm at 7-84 days and 0.0067 ppm at 298 days. The degradate PCB was detected at 0.072-0.011 ppm at 1 and 14 days posttreatment in the 6- to 12- and 12- to 18-inch soil depths, and at 0.010 ppm at 14 days in the 18- to 24-inch depth. PCA was detected at 0.0071 ppm at 126 days in the 6- to 12-inch depth, was not detected (<0.005 ppm) in the 12- to 18-inch depth, and was detected at 0.011 ppm at 298 days in the 18- to 24-inch depth. PCTA and HCB were not detected (<0.005 ppm) at any depth below 6 inches.

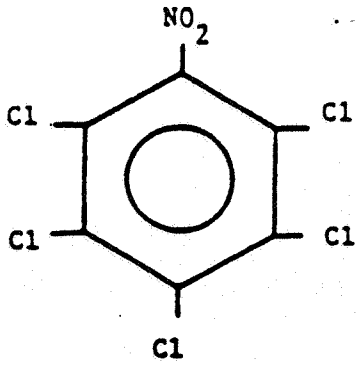
During the study, rainfall totaled 24.47 inches and air temperatures ranged from -29 to 104°F. The depth to the water table was approximately 20 feet, and the slope of the field was <1%.

COMMENTS:

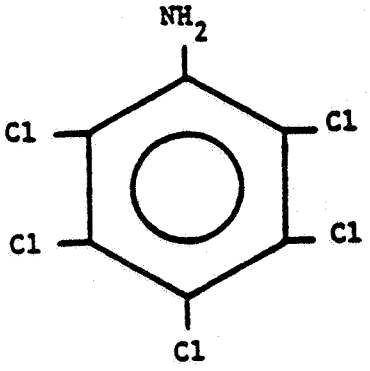
1. The study author stated that the isolated incidents of residues detected below the 0- to 6-inch soil layer were believed to be the result of contamination rather than leaching. This may be the case for the isolated detections of PCB and PCA; however, PCNB was detected below the 0- to 6-inch depth at several intervals, and it could not be determined if PCNB had leached from the surface layer or was present because of poor sampling techniques.

2. Soil temperatures were not provided.

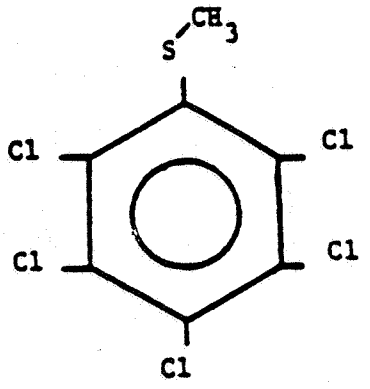
Chemical Structures of PCNB, PCA, PCTA, PCB and HCB



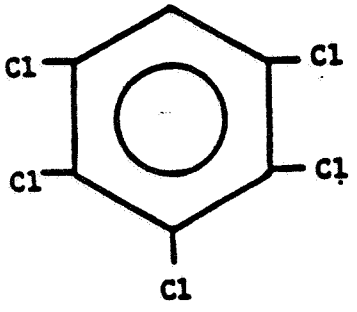
PCNB (Pentachloronitrobenzene)



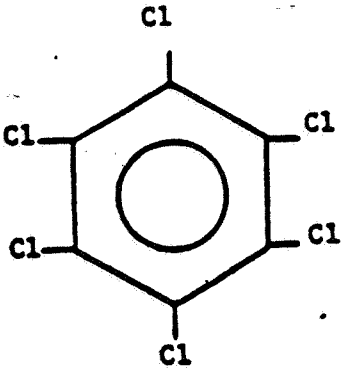
PCA (Pentachloroaniline)



PCTA (Pentachlorothioanisole)



PCB (Pentachlorobenzene)



HCB (Hexachlorobenzene)

PCNB environmental fate review

Page _____ is not included in this copy.

Pages 125 through 135 are not included in this copy.

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 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

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X FIFRA registration data

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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.

DATA EVALUATION RECORD

STUDY 10

CHEM 056502 Pentachloronitrobenzene §164-1

FORMULATION--04--GRANULAR (G)
STUDY ID 41313501

Rice, F., B. Jacobson, and M.W. Winberry. 1989. Terrestrial field dissipation for PCNB in peanuts. Uniroyal Project No. 8754A. Unpublished study performed by Southern Agricultural Research, Inc., Donalsonville, GA and Analytical Bio-Chemistry Laboratories, Inc., Columbia, MO; and submitted by Uniroyal Chemical Co., Inc., Middlebury, CT.

This study was previously reviewed by EFGWB on June 27, 1990.

DATA EVALUATION RECORD

STUDY 11

CHEM 056502 Pentachloronitrobenzene §165-1

FORMULATION--00--ACTIVE INGREDIENT

STUDY ID 41562905
Halls, T.D.J. 1990. Confined accumulation of ^{14}C-PCNB on rotational crops treatment, sampling and combustion analysis. Uniroyal Project No. 8755. ABC Laboratories Final Report No. 35971. Unpublished study performed by Analytical Bio-chemistry Laboratories, Columbia, MO; and submitted by Uniroyal Chemical Company, Incorporated, Middlebury, CT.

DIRECT REVIEW TIME = 10

REVIEWED BY: W. Martin TITLE: Staff Scientist

EDITED BY: T. Colvin-Snyder TITLE: Staff Scientist
K. Patten Task Leader

APPROVED BY: W. Spangler TITLE: Project Manager

ORG: Dynamac Corporation
Rockville, MD

SECONDARY REVIEW BY: D. Spatz
TITLE: Chemist
ORG: EFGWB/EFED/OPP

SIGNATURE: DEC 28 1990

CONCLUSIONS:

Confined Accumulation - Rotational Crops

1. This study cannot be used to fulfill the Confined Accumulation in Rotational Crops data requirement at this time.

2. Uncharacterized [^{14}C]pentachloronitrobenzene (PCNB) residues accumulated in lettuce, turnips, and wheat that were planted in sheltered outdoor plots of fine sandy loam soil at 30, 120, and 365 days after the soil was treated with [^{14}C]PCNB (radiochemical purity 100%) plus unlabelled PCNB (purity 99.2%) at 30 lb ai/A.

   In immature wheat, PCNB residues were 2.59 and 5.05 ppm in wheat planted at 30 and 365 days posttreatment, respectively. In the mature wheat straw, PCNB residues were 22.2-25.9 ppm; in the mature wheat hulls, PCNB residues were 6.06-11.1 ppm; and in the grain, PCNB residues were 0.332-0.710 ppm.

In immature turnips, PCNB residues were 4.61 and 1.60 ppm in turnips planted at 30 and 365 days posttreatment, respectively. In mature turnip greens, PCNB residues were 3.63 ppm in turnips planted at 30 days posttreatment and 0.727 ppm in turnips planted at 365 days. In mature turnip roots, PCNB residues were 20.3 ppm in turnips planted at 30 days posttreatment and 1.48 ppm in turnips planted at 365 days.

In immature lettuce, PCNB residues were 1.40-5.67 ppm. In mature lettuce PCNB residues were 0.146-1.62 ppm.

In the upper 6 inches of the soil, uncharacterized PCNB residues were 6.56-14.3 ppm at 2 hours posttreatment, 8.41-12.6 ppm at 30 days, 5.89-8.02 ppm at 120 days, 4.84-6.52 ppm at 365 days, and 4.84-5.61 ppm at 426-472 days. PCNB residues were sporadically recovered at 0.024-1.05 ppm in the 6- to 12-inch soil layer.

3. This study is <u>not acceptable</u> for the following reasons:

   a. The PCNB residues in the plant tissue and soil samples were not characterized. The samples were analyzed only for total radioactive residues.

   b. The length of freezer storage of crop and soil samples prior to analysis was not reported, and no freezer storage stability data were provided.

   c. Material balances and supporting raw data were not provided.

   d. The application rate was not confirmed by the immediately post-application residue measurement. At an application rate of 30 lbs ai/acre, there should have been ≈15 ppm in the soil (6-inch depth). However, the 2-hour post-application sampling showed that none of the plots reached 15 ppm in the soil and many of them measured below 10 ppm.

4. Although ^{14}C-residues were found in all three crops planted 30, 120, and 365 days posttreatment; because these residues were not characterized, a Field Accumulation in Rotational Crops study would not be appropriate at this time. The authors stated that residue analysis was in progress. Confirmatory residue identification, material balances, and storage stability data must be submitted for this study. Once these data are submitted and if found acceptable, then a decision can be made to either conduct a Field Accumulation study for the purpose of setting a rotational interval or, petition for tolerances. If the supporting data are not found to be acceptable, a new confined accumulation study will be required.

METHODOLOGY:

The test site (30 x 60 feet) was surrounded by fencing and covered with a corrugated fiberglass roof. During the winter, the test site was enclosed in polyethylene sheeting and heated by gas furnaces; additional illumination was provided by fluorescent "grow lights". Within this sheltered test site, six test plots were created by filling polyethylene-lined, fiberglass-coated metal containers (each 3 x 8 feet, 18-inch depth) with 18 inches of non-indigenous fine sandy loam soil (56% sand, 32% silt, 12% clay, pH 8.1, CEC 9.4 meq/100 g, organic matter content not reported). Each container/plot was further divided into three subplots using steel cylinders cut from a 55-gallon drum (Figure 1).

Uniformly ring-labeled [^{14}C]pentachloronitrobenzene (PCNB; radiochemical purity 100%, specific activity 2490 dpm/μg, source not reported) plus unlabeled PCNB (purity 99.2%, source not reported) were applied at 30 lbs ai/A to each subplot in three of the treatment plots on May 11, 1988, using a carbon dioxide sprayer. After each application, the spray system was rinsed twice with acetone and once with methanol; the rinses were applied to the subplot. Immediately after application, the PCNB was incorporated into the upper 2-4 inches by hand cultivation. The remaining three plots were left untreated to serve as controls.

A target cabbage crop was planted in the 120 and 365 day test plots 30 days posttreatment to mimic an actual field-use situation. At 30, 120, and 365 days posttreatment, the subplots were planted to lettuce, turnips, or wheat. Immature plant samples were collected by thinning the crop, and mature samples were collected by harvesting all of the plants within a subplot. Immature plant samples, mature lettuce, and mature wheat consisted of the entire aerial portion of the plants; mature turnips were divided into tops and roots; and mature wheat was divided into straw, grain and hull portions. The samples were homogenized in dry ice and stored frozen at -20°C for an unspecified period of time prior to analysis.

Soil samples were collected before treatment, at 2 hours posttreatment, and at all rotational crop planting and harvest intervals. Single 12-inch soil cores were taken in the untreated controls, and triplicate samples were collected in the treated subplots. The soil cores were frozen immediately after collection and divided into 0- to 6- and 6- to 12-inch segments. Samples from the same treatment, sampling interval, and depth were composited in dry ice and stored frozen at -20°C for an unspecified period of time prior to analysis.

Triplicate subsamples of the plant tissues and soil were analyzed by LSC following combustion. Recoveries from the plant tissue subsamples were 86.1-100%; recoveries from the soil subsamples were 93.2-97.5%.

COMMENTS:

1. The organic matter content of the soil was not reported.

2. The author stated that wheat samples from the control plot planted at 120 days posttreatment contained radiocarbon (concentration not reported). The study author attributed the presence of radiocarbon in these samples to the utilization of [^{14}C]carbon dioxide generated by the plants in the treated plot which was trapped in the enclosed shelter.

3. The recovery of [^{14}C]residues in the 6- to 12-inch soil layer was attributed by the study author to contamination from the 0- to 6-inch soil layer.

4. During the study, the plots were fertilized and treated with diazinon and Sevin. The wheat was also treated with carbofuran, captan, acephate and propiconazole; the turnips were treated with insecticidal soap; and the lettuce and turnips were treated with Bacillus thuringiensis.

PCNB environmental fate review

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DATA EVALUATION RECORD

STUDY 12

CHEM 056502 Pentachloronitrobenzene §165-4

FORMULATION--00--ACTIVE INGREDIENT

STUDY ID 40580202
Forbis, A.D. 1988. Uptake, depuration, and bioconcentration of ^{14}C-PCNB to bluegill sunfish (Lepomis macrochirus). Laboratory Project ID ABC #35965. Unpublished study performed by Analytical Bio-Chemistry Laboratories, Columbia, MO, and submitted by Uniroyal Chemical Company, Middlebury, CT.

DIRECT REVIEW TIME = 8

REVIEWED BY: N. Glassbrook TITLE: Staff Scientist

EDITED BY: T. Colvin-Snyder TITLE: Staff Scientist
K. Patten Task Leader

APPROVED BY: W. Spangler TITLE: Project Manager

ORG: Dynamac Corporation
Rockville, MD

SECONDARY REVIEW BY: D. Spatz
TITLE: Chemist
ORG: EFGWB/EFED/OPP

SIGNATURE: DEC 28 1990

CONCLUSIONS:

Laboratory Accumulation - Fish

1. This study cannot be used to fulfill the Bioaccumulation in Fish data requirement at this time.

2. Uncharacterized pentachloronitrobenzene (PCNB) residues accumulated in bluegill sunfish exposed to [^{14}C]PCNB at a mean concentration of 0.54 ppb for 28 days. Maximum mean bioconcentration factors were 370x for edible tissues, 1800x for viscera, and 960x for whole fish. At the end of the 21-day depuration period, 81-84% of the accumulated [^{14}C]residues were eliminated from the fish tissues.

3. This study is scientifically sound and provides supplemental information, but does not meet Subdivision N guidelines for the following reason:

> Radioactive residues in the water and fish tissues were not characterized. Fish samples were collected on days 21 and 28 of exposure and on day 14 of depuration for "metabolite characterization", but the results of these analyses were not presented in this study.

4. In order for this study to fulfill the accumulation in laboratory fish data requirement, data confirming the identification of PCNB residues in the water and fish tissues and supporting storage stability data must be submitted.

METHODOLOGY:

Flow-through aquatic exposure systems were prepared using two 100-L aquaria containing approximately 70 L of aerated well water (pH 8.1-8.4, dissolved oxygen content 7.0-8.9 mg/L; additional water characteristics presented in Table 1). Aerated water was intermittently supplied to each aquarium at an average flow rate of 380 mL/minute, equivalent to 7.9 turnovers per day. One of the aquaria was treated intermittently using a proportional dilution system with a solution of [^{14}C]pentachloronitrobenzene (PCNB; radiochemical purity 98%, specific activity 29.8 μCi/mg, Uniroyal) in acetone at a nominal concentration of 0.70 ppb PCNB; the other aquarium was treated with an equal amount of pesticide-free acetone. The aquaria were immersed in a water bath maintained at 22 ± 2°C and allowed to equilibrate for 24 hours before the introduction of fish.

Bluegill sunfish (Lepomis macrochirus, mean length 59 mm, mean weight 7.6 g) were held in culture tanks on a 16-hour photoperiod for 14 days prior to the initiation of the study. At the start of the exposure period, 120 acclimated fish were placed in each of the two aquaria. The fish were fed a commercial fish food daily in amounts equivalent to approximately 3% of their body weight. Following a 28-day exposure period, the water in the aquaria was twice siphoned off to a depth of 8 cm and replaced with approximately 70 L of untreated well water. The fish were maintained in the aquaria for a 21-day depuration period during which the flow-through system was maintained using untreated water. Fish and water samples were taken from each aquarium immediately prior to the introduction of fish to the aquaria and after 0.17, 1, 3, 7, 14, 21, and 28 days of exposure.

Radioactivity in the water was quantified using LSC. Three fish from each sampling interval were dissected into edible (body, muscle, skin, and skeleton) and visceral (fins, head, and internal organs) portions. Dissected and whole fish were stored frozen for an

unspecified period of time until analysis. Samples of pooled edible and nonedible tissues along with three additional whole fish samples were analyzed for total radioactivity following combustion. Recovery efficiencies from [^{14}C]PCNB-fortified edible, visceral, and whole fish samples ranged from 96% to 101%. Minimum quantifiable concentrations of PCNB residues were 0.0439, 1.94, 1.97, and 2.04 ppb PCNB equivalents for water, edible, whole fish, and viscera, respectively.

DATA SUMMARY:

Uncharacterized pentachloronitrobenzene (PCNB) residues accumulated in bluegill sunfish exposed to [^{14}C]PCNB (radiochemical purity 98%) at a nominal concentration of 0.70 ppb for 28 days under flow-through conditions. The maximum mean bioconcentration factors were 370x for edible tissues, 1800x for viscera, and 960x for whole fish. Maximum mean concentrations of total [^{14}C]residues were 200 ppb at 21 days for edible tissue, 990 ppb at 28 days for viscera, and 520 ppb at 21-28 days for whole fish. The mean concentration of [^{14}C]PCNB residues in the water was 0.54 ppb PCNB equivalents. After 21 days of depuration, 81% of the accumulated [^{14}C]residues were eliminated from edible tissue, 84% were eliminated from viscera, and 83% were eliminated from whole fish.

Total [^{14}C]PCNB residues in the treated water ranged from 0.31 to 0.67 ppb. Over the course of the study, daily water temperatures were constant at 21°C.

COMMENTS:

1. A preliminary 14-day toxicity study was conducted to determine the acute toxicity of PCNB to bluegill sunfish. The 14-day LC_{50} value was 66 ppb after 14 days and the no-effect concentration was 22 ppb. The authors chose 0.70 ppb for the exposure level, which was a factor of 94 below the LC_{50}.

2. No abnormal behavior or mortality was observed in the fish during the study.

3. Bioconcentration of ^{14}C-PCNB residues in the viscera did not plateau during the 28-day exposure period.

4. The study author stated that the water and the test substance were supplied "intermittently" rather than continuously as is usually done in laboratory fish studies. The average water flow rate of 380 mL/minute and the turnover rate of 7.9 turnovers per day are typical of continuous flow-through conditions.

PCNB environmental fate review

Page _____ is not included in this copy.

Pages 158 through 162 are not included in this copy.

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DATA EVALUATION RECORD

STUDY 13

CHEM 056502 Pentachloronitrobenzene §165-5

FORMULATION--12-EMULSIFIABLE CONCENTRATE (EC)

STUDY ID 41521001
Forbis, A.D. 1990. Bioconcentration of ^{14}C-PCNB to channel catfish (Ictalurus punctatus) and bluegill (Lepomis macrochirus) under static uptake conditions. ABC Final Report No. 37033. Unpublished study performed by Analytical Bio-Chemistry Laboratories, Columbia, MO, and submitted by AMVAC Chemical Corporation, Los Angeles, CA.

DIRECT REVIEW TIME = 10

REVIEWED BY: N. Glassbrook TITLE: Staff Scientist

EDITED BY: T. Colvin-Snyder TITLE: Staff Scientist
K. Patten Task Leader

APPROVED BY: W. Spangler TITLE: Project Manager

ORG: Dynamac Corporation
Rockville, MD

SECONDARY REVIEW BY: D. Spatz
TITLE: Chemist
ORG: EFGWB/EFED/OPP

SIGNATURE: DEC 28 1990

CONCLUSIONS:

Field Accumulation - Aquatic Nontarget Organisms

1. This study is not acceptable for the following reasons:

   a. Residues in the fish tissues, water, and soil were not characterized.

   b. At 28 days posttreatment, approximately 29% of the applied radioactivity was unaccounted for.

2. Uncharacterized pentachloronitrobenzene (PCNB) residues accumulated in channel catfish and bluegill sunfish maintained under simulated field conditions for 28 days in water treated with a single application of PCNB at 0.10 ppm. The maximum mean bioconcentration factors for channel catfish were 250x in the edible tissues, 630x in the visceral tissues, and 460x in the whole fish; the maximum mean

bioconcentration factors for bluegill sunfish were 120x in the edible tissues, 560x in the visceral tissues, and 330x in the whole fish.

3. The PCNB Registration Standard (January 1987), inadvertently required an Accumulation in Aquatic Non-Target Organisms study. However, under the presently registered uses of PCNB (terrestrial food and non-food), this study is not required. The Ecological Effects Branch of EFED was consulted on this matter, (Allen Vaughan, 1/5/88), and their conclusions were in agreement with those of EFGWB. Although PCNB does bioconcentrate in fish tissue, there is appreciable depuration. At the present time and with the currently registered uses, an Accumulation in Aquatic Non-Target Organisms study is not required.

METHODOLOGY:

Channel catfish (Ictalurus punctatus; mean length 96 mm; mean weight 14.5 g) and bluegill sunfish (Lepomis macrochirus; mean length 59 mm; mean weight 7.6 g) were held in culture tanks on a 16-hour daylight photoperiod for ≥14 days prior to initiation of the study. Outdoor aquatic static exposure systems were prepared using 1500-L fiberglass-lined fish tanks containing approximately 1300 L of aerated well water (pH 7.6-8.7, dissolved oxygen content 5.8-15.8 mg/L; additional water characteristics presented in Table 2) and 100 kg of sandy loam soil (56% sand, 32% silt, 12% clay, 1% organic matter, pH 8.1, CEC 9.4 meq/100 g). Aeration was provided by continuously circulating water between the fish tanks and a 500-L mixing tank at approximately 200 L/hr. The exposure systems were placed outdoors in an open-air greenhouse in Boone County, Missouri, for 28 days during September and October under natural sunlight moderated with shade cloth to limit heating of the water. During the study, the water temperatures ranged from 8-25°C. At 14 days after establishing the test system, the fish were placed in the fish tanks and allowed to acclimate for 10 days. During the study, the fish were fed a commercial fish food in amounts equivalent to approximately 3% of their body weight per day.

A mixture of uniformly ring-labeled [^{14}C]pentachloronitrobenzene (PCNB, radiochemical purity 99%, specific activity 12.2 mCi/mmol, source not specified) plus nonradiolabeled, formulated PCNB (PCNB 2E, 2 lb/gal EC, AMVAC), dissolved in acetone, were added once in a single application to the mixing and fish tanks at a nominal concentration of 0.10 ppm. Fish and water were sampled immediately before treatment and at 0.17, 1, 3, 7, 14, 21, and 28 days posttreatment. Soil was sampled at 28 days posttreatment. Radioactivity in the water was quantified using LSC. Twelve fish of each species were collected at each sampling interval. Eight fish of each species were dissected into edible (body, muscle, skin, and skeleton), and viscera (fins, head, and internal organs) portions; the remaining four fish were analyzed as whole fish samples. Soil and fish tissues were analyzed for total radioactivity by LSC following combustion. Recovery efficiencies from [^{14}C]PCNB-fortified

edible, visceral, and whole fish samples ranged from 97% to 101%. Minimum quantifiable concentrations of PCNB residues were 0.0002 ppm PCNB equivalents for water and were 0.130-0.153 ppm PCNB equivalents for soil and fish samples.

DATA SUMMARY:

Uncharacterized [^{14}C]pentachloronitrobenzene (PCNB) residues accumulated in channel catfish and bluegill sunfish maintained under simulated field conditions for 28 days in water treated at 0.10 ppm with a single application of [^{14}C]PCNB (radiochemical purity 99%) plus formulated nonradiolabeled PCNB (PCNB 2E, 2 lb/gal EC). The maximum mean bioconcentration factors for channel catfish were 250x in the edible tissues, 630x in the visceral tissues, and 460x in the whole fish; the maximum mean bioconcentration factors for bluegill sunfish were 120x in the edible tissues, 560x in the visceral tissues, and 330x in the whole fish. Maximum mean concentrations of total [^{14}C]PCNB residues in channel catfish were 15 ppm for edible tissue, 43 ppm for viscera, and 31 ppm for whole fish at day 1 posttreatment. Maximum mean concentrations of total [^{14}C]PCNB residues in bluegill sunfish were 6.8 ppm at 7 days for edible tissue, 39 ppm at 1 day posttreatment for viscera, and 23 ppm at day 1 posttreatment for whole fish.

Total [^{14}C]PCNB residues in the treated water decreased from 0.08 ppm at 0.17 days posttreatment to 0.034 ppm by 28 days posttreatment. [^{14}C]PCNB residues in the soil were 0.380 ppm in the catfish tank and 0.510 ppm in the bluegill tank at 28 days posttreatment.

By 28 days posttreatment, 34% of the applied activity was in the water, 29% was in the soil, and 8% had accumulated in fish tissue; the remaining 29% was assumed to be adsorbed to the test system or lost by volatilization.

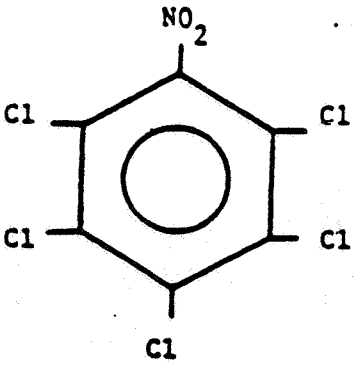
COMMENTS:

1. PCNB residues in fish tissues, water, and soil were not characterized. The study author stated that characterization of PCNB residues in fish tissues and freezer storage stability data will be submitted at a later date.

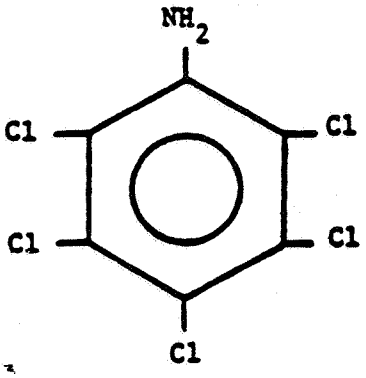
2. A concentration of 0.10 ppm PCNB was chosen based on the difficulty of dissolving PCNB in test water and the observed mortality of fish at 200 ppb.

3. Bioconcentration of PCNB residues in catfish did not plateau.

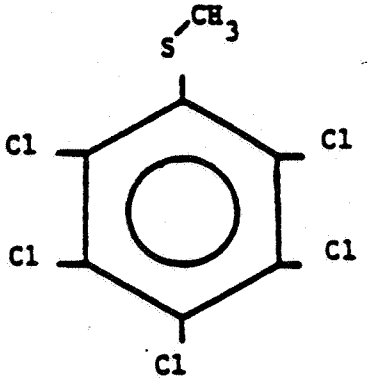
Chemical Structures of PCNB, PCA, PCTA, PCB and HCB



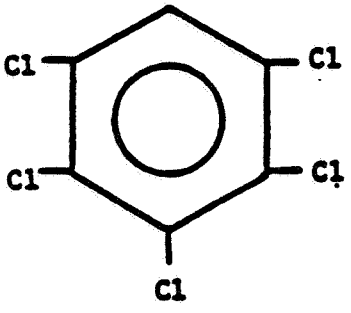
PCNB (Pentachloronitrobenzene)



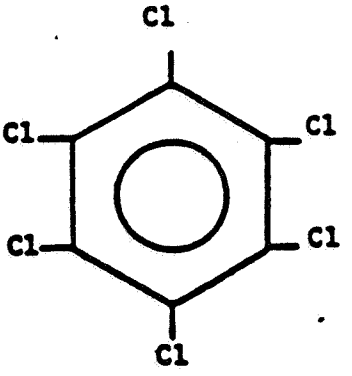
PCA (Pentachloroaniline)



PCTA (Pentachlorothioanisole)



PCB (Pentachlorobenzene)



HCB (Hexachlorobenzene)

PCNB environmental fate review

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