SUMMARY

PCNB and its degradates were extracted from soil. Before analysis one of the degradates, pentachlorophenol, was converted to the methyl ether using diazomethane. The combined extracts were analyzed by GC using an electron capture detector.

A) MATERIALS

A.1 Equipment

Balance
Centrifuge
Centrifuge bottle, teflon 250 ml
Hobart Food Chopper
Erlenmeyer Flask, 250 ml
pH meter
Rotary evaporator, Buchi Rotovap
Round bottom flasks, 500 ml
Separatory funnel, 250 ml
Standard laboratory equipment:
  beakers, pipets, test tubes etc.
TurboVap LV evaporator

Mettler PE 3000
Damon/IEC
Nalgene
Hobart Mfg. Co.
Pyrex, Kimax
Beckman
Brinkman
Pyrex, Kimax
Nalgene
Pyrex, Kimex
Zymark

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A.2 Reagents/Supplies

Acetone, residue grade
1-Decanol
Diazomethane in diethyl ether solution
Diethyl ether, residue grade
Dry Ice
n-Hexane, residue grade
HCB Analytical Standard AC-1194-38C
Nitrogen
PCA Analytical Standard AC-1234-1
PCB Analytical Standard AC-1166-14
PCNB Analytical Standard AC-1261-133
PCP Analytical Standard AC-1261-84
PCTA Analytical Standard AC-1166-16
PCTASO Analytical Standard AGD-1384-005
Sodium Hydroxide
Sulfuric Acid
TCTASOO Analytical Standard AGD-1384-024
Toluene, residue grade

Baker
Baker
Aldrich
Baker
Penn State University
Baker
Uniroyal Chemical Co.
MG Industries
Uniroyal Chemical Co.
Uniroyal Chemical Co.
Uniroyal Chemical Co.
Uniroyal Chemical Co.
Uniroyal Chemical Co.
Baker
Baker
Uniroyal Chemical Co.
Baker

A.3 Analytical Standards

The following standards are used to analyze for PCNB and its degradates. Standards should be stored at -5°C to -25°C until use. Standards can be obtained from Uniroyal Chemical Inc. Structures for these standards are shown in Figure I.
<table>
<thead>
<tr>
<th>NAME</th>
<th>LOT NUMBER</th>
<th>PURITY</th>
</tr>
</thead>
<tbody>
<tr>
<td>PCNB</td>
<td>AC-1261-133</td>
<td>99.8%</td>
</tr>
<tr>
<td>PCB</td>
<td>AC-1166-14</td>
<td>100.0%</td>
</tr>
<tr>
<td>HCB</td>
<td>AC-1194-38C</td>
<td>99.8%</td>
</tr>
<tr>
<td>PCA</td>
<td>AC-1234-1</td>
<td>97.0%</td>
</tr>
<tr>
<td>PCTA</td>
<td>AC-1166-16</td>
<td>99.1%</td>
</tr>
<tr>
<td>PCP</td>
<td>AC-1261-84</td>
<td>98.4%</td>
</tr>
<tr>
<td>TCTASOO</td>
<td>AGD-1384-024</td>
<td>99.4%</td>
</tr>
<tr>
<td>PCTASO</td>
<td>AGD-1384-005</td>
<td>96.7%</td>
</tr>
</tbody>
</table>

MSDS sheets for the above standards are found in Appendix I.

**B. SAFETY AND HEALTH**

This method should be performed by trained chemical personnel. Hazards associated with the chemicals used in this analytical method are shown in the MSDS sheets in Appendix I. Special precautions are needed during the use of diazomethane.

**C. ANALYTICAL METHOD**

**C.1 Principle of the Method**

Soil samples are homogenized and then extracted with acetone/hexane. Basic and neutral degradates (and PCNB) are partitioned into hexane after addition of pH 12 water. PCP is partitioned from the water phase into hexane after acidification and methylated with diazomethane. Both organic extracts are then
combined and the components analyzed by GC using an electron capture detector.

C.2 Types of Soils

This method is predicted to be applicable to most soil types. In Uniroyal Chemical Inc. project 92147 soils from a Texas USA location were used and the composition varied depending on soil depth from sandy loam (0-12 inch depth) to sandy clay loam (12-24 inch depth) to clay loam (24 to 48 inch depth).

C.3 Sample Processing

Frozen cores are normally received and are divided into smaller pieces with a cleaver and rubber mallet. The stones and debris are removed. A Hobart Food Chopper is pre-chilled with dry ice and the frozen soil pieces are put inside. The soil is chopped and homogenized with dry ice. The processed soil is placed in sample containers and stored in the freezer where the dry ice is allowed to sublime overnight at < -10°C. The sample containers are capped and kept under freezer conditions (-5°C to -25°C) until analysis.

C.4 Extraction Method

A flow diagram of the analysis procedure is shown in Figure II. Detailed explanations of each step are as follows:

**Step 1** Extraction (10 g soil, wet weight)

Weigh 10 g of soil in a 250 ml teflon centrifuge bottle. Fortify the two spike samples used to determine extraction method recoveries for the set of samples.
Add 100 ml 50:50 v/v acetone: hexane and shake vigorously for 2 min. Centrifuge at 1500 RPM for 5 min. Pour the supernatant into a separatory funnel, leaving the soil in the bottle. Add another 50 ml of 50:50 v/v acetone: hexane to the soil, shake 1 min and centrifuge. Add supernatant to the separatory funnel.

**Step 2**  
**Partition**

Add 50 ml distilled/deionized water (pH > 12, adjusted with 25% NaOH) to the separatory funnel and shake for 20 sec. Drain the water/acetone layer into a 250 ml beaker and collect the hexane layer in a 250 ml Erlenmeyer flask. Re-extract the water/acetone layer with 50 ml hexane, shaking for 1 min. Drain the water/acetone layer into the 250 ml beaker and add the remaining hexane layer to the flask. The extract done under basic conditions, in the Erlenmeyer flask, contains compounds PCB, HCB, PCNB, PCA, PCTA, TCTASOO, and PCTASO.

**Step 3**  
**Removal of Acidic Metabolite**

Pour the water/acetone portion back into the separatory funnel and add 10 ml 10N H₂SO₄ to lower the pH < 1. Add 50 ml hexane, shake vigorously for 1 min and drain the water/acetone layer into the beaker. Pour the hexane layer into a 500 ml round bottom flask. Re-extract the water/acetone with another 50 ml hexane by shaking for 1 min. Drain the water/acetone layer into the beaker and add the remaining hexane layer to the round bottom flask. The extract done under acidic conditions, in the round bottom flask, contains the compound PCP.

**Step 4**  
**Methylation, Diazomethane Method**
Add 10 drops of decanol to the acidic extract to prevent the sample from going to dryness during evaporation and reduce the volume to about 5 ml using a rotary evaporator. Transfer this portion of the sample into a methylation vial, rinsing the round bottom flask with hexane. Further reduce the volume of the sample to 0.5 ml using a TurboVap LV evaporator under nitrogen. Add 0.5 ml diazomethane, or enough to turn the sample yellow. Let it stand under a hood for 10 min. Evaporate off the diazomethane using the TurboVap, reducing the volume again to 0.5 ml.

Step 5 Combine the Extracts and Adjust the Volume

Rinse a round bottom flask with acetone and transfer the basic extract (prepared in Step 2) from the Erlenmeyer flask to the round bottom flask. Reduce the volume to about 5 ml using the rotary evaporator, then add 10 ml toluene. Pour the methylated portion of the sample into the round bottom flask, rinsing the vial with 15 ml toluene. Reduce the volume of the combined extracts to about 5 ml with the rotary evaporator, then and bring the final volume up to 10 ml with toluene. The sample is now ready for GC analysis.

Step 6 Percent Soil Moisture Determination

Percent soil moisture is determined by weighing two aliquots of soil, before and again after oven drying for 16 hours at 100°C.

C.5 Gas Chromatography Method

The type of column used in the GC analysis of soil samples is a Restek Rtx-35, 30 meter in length, 0.53 mm internal diameter (ID), with 0.25 μm film thickness (DF). The Rtx-35 has a stationary phase made of 35% diphenyl-65%
dimethyl polysiloxane. It is rated intermediate in polarity. The samples are delivered to the column by direct injection. The injector temperature is 270°C. The column housing oven is programmed to increase the temperature at a rate of 5°C/min from 100°C to 200°C, during which all of the compounds of interest passed through the column to the ECD detector. This is followed by a temperature increase at 20°C/min to 270°C to clean out any remaining impurities. The detector temperature is set at 300°C.

The GC run begins with the injection of a 1 μl aliquot of each of the four eight-component mixed standards in the range of 0.003μg/ml to 0.100 μg/ml. Standards and washes are run intermittently with the samples to help monitor the stability of the run, and to make sure the column is clean before the next sample is injected. The resulting standard peak areas are plotted versus concentration (μg/ml) of the corresponding standard to obtain standard calibration curves. Standard curves are generated for each analysis day, using all standards injected during the run.

A 1 μl aliquot of the sample is injected into the GC. If the compound peak area in the sample is greater than the peak area of the highest standard, the sample extract is diluted with toluene until the signal response falls within the standard curve range. The peak areas of the compounds are recorded and the concentration of each compound is determined relative to the standard curves generated for that day.

C.6 Preparation of Spiking and Standard Solutions

Analytical standards are used to prepare individual compound stock solutions from which working standard and method day spiking solutions are prepared. Stock solutions of each compound at a concentration of 1.0 mg/ml are made by
weighing out 10 mg of the analytical standard on an analytical balance and
dissolving it in 10 ml of toluene. The amount of toluene added is determined
considering the percent purity of the standard. For example, PCTA was 99.1%
pure, so 10 mg of PCTA is weighed out and dissolved in 9.91 ml of toluene
(10.0 x 0.991). The PCP stock solution is prepared using methanol.
Methylated pentachlorophenol (PCP-OME) is prepared in toluene and corrected
considering the PCP equivalence. The molecular weight of PCP (266) is
divided by the molecular weight of PCP-OME (280) to yield a correction factor
of 0.95. For example, if 10.0 mg of PCP-OME is weighed out, then 9.50 ml of
toluene is added to make 1 mg/ml solution (10.0 x 0.95 = 9.50).

A solution of seven compounds combined in toluene at a concentration of 100
μg/ml is made by adding 2 ml of each of the individual compound stock
solutions at 1.0 mg/ml of PCB, HCB, PCNB, PCA, PCTA, TCTASOO and
PCTASO, to 6 ml of toluene, so that the final volume is 20 ml. A solution of
PCP at 100 μg/ml is made by diluting the 1.0 mg/ml stock solution of PCP 10-
fold with methanol.

A method spiking solution of the combined seven compounds at a concentration
of 10 μg/ml is made by a 10-fold dilution of the 100 μg/ml seven compound
solution with toluene. Likewise, a PCP spiking solution at 10 μg/ml is made by
a ten fold dilution with methanol of the 100 μg/ml PCP solution. Fortification
of the method spike samples at a 0.1 ppm level is accomplished by adding 100
μ1 of the 10 μg/ml spiking solutions to 10 g. of control soil, and bringing the
final volume of the extract to 10 ml. Fortification of the method spike samples
at a 1.0 ppm level is done by adding 100 μ1 of the 100 μg/ml spiking solutions
to 10 g of control soil and bringing the final volume of the extract to 10 ml.

A 10 μg/ml standard solution is made by adding 200 μ1 of each individual
compound stock solutions of PCB, HCB, PCP, PCNB, PCA, PCTA, TCTASOO and PCTASO at 1 mg/ml, and bringing the final volume to 20 ml with toluene. In this case the solution of PCP-OMe in toluene is used. A 1 μg/ml standard solution of the combined eight compounds is prepared by diluting the 10 μg/ml standard solution 10 fold with toluene. Dilutions of the 10 μg/ml and 1 μg/ml standard stock solutions are made to prepare working standards at 0.100 μg/ml, 0.050 μg/ml, 0.010 μg/ml, and 0.003 μg/ml.

C.7 Extraction Efficiency

Duplicate soil samples were spiked in the field with each of the analytes PCNB, PCA, PCP, PCTA, PCB, HCB, PCTASO and TCTASOO on two occasions, at the 120 day sampling (0-3 month) and at the 270 day sampling (6-12 month). The results of spiking at a level of 1.0 μg of analyte in 10 g of soil are shown in Table VI of Uniroyal Project 92147 (Figure III of this report). These results indicate that the analytes did not undergo significant breakdown under the conditions of handling and shipping. Examples of chromatograms and data calculation spreadsheets for the field spikes are presented in Appendix II.

C.8 Fortifications

Soil samples spiked in the laboratory which were extracted and analyzed along with the actual test samples showed recoveries in the range of 70 – 120% for all of the analytes. The laboratory spike results indicate that the analytical methodology provided reliable results during the course of study 92147. An example of chromatograms of control samples and spiked control samples are shown in Appendix III (taken from studies 92147 and RP 91051).
D. **INSTRUMENTATION**

The gas chromatograph and integrator models, column type, and operating conditions were as follows:

**Instrument:** Hewlett Packard Model 5890 Series II Gas Chromatograph  
**Column:** Restek RTX-35, 30 m, 0.53 mm ID, 0.25 um df  
**Oven:**  
  - Initial temp. 100°C, Initial time 2 min  
  - Rate A: 5°C/min to 200°C, final time 1 min  
  - Rate B: 20°C/min to 270°C, final time 5 min  
**Detector:** Electron Capture Detector (ECD), temp. 300°C  
**Injector:** Direct Injection, temp. 270°C  
**Carrier Gas Flow:** Hydrogen, 10 ml/min  
**Make-up Flow:** Nitrogen, 35 ml/min  
**Integrator:** Shimadzu C-4RA Chromatopac

E. **SAMPLE BRACKETING**

The calibration was done by standard bracketing. A typical run involved running the standard curve, followed by a control, then two day spikes, 4 samples, two day spikes, and 4 more samples. Data from a typical run including the chromatographs are shown in Appendix IV.

F. **POTENTIAL INTERFERENCES**

This method could have interferences from other halogenated pesticides that might elute with similar retention times. One should consider the soil history in this respect and a confirmatory technique should be used if a problem is suspected.
G. **CONFIRMATORY TECHNIQUES**

The method of confirmation for the definite identification of PCB, HCB, PCNB, PCA, PCTA, TCTASOO and PCTASO was by GC/MS. It was completed using two standard solutions and sample 932265, which gave sharp peaks for all of the compounds of interest except PCP. The base peaks used in the spectra for selective ion monitoring of the compounds in the samples is as follows: compound-base peak, qualifying peak PCB-250, 215, HCB-284, 249, PCNB-237, 295, PCA-265, 263, PCTA-296, 246, TCTASOO-231, 215, PCTASO-297, 295. Comparing the total ion chromatograms of standard solutions containing all eight compounds at 0.100, 0.050 µg/ml the order of elution of the compounds is shown to be PCB, HCB, PCP, PCNB, PCA, PCTA, TCTASOO, PCTASO. Chromatograms showing these confirmations are shown in Appendix V.

The method of confirmation for the definite identification of PCP was done using an RXT-200 chromatographic column. The level of this compound found in the samples is usually too low for detection by GC/MS. Samples which show the greatest amount of this compound can be used for the confirmation. The RTX-200 column has a polarity selective for lone pair electrons and gives a sharp PCP peak. Confirmation of PCP can thus be done using the RTX-200 column rather than the RTX-35 column as a second chromatographic technique. Typical chromatograms of PCP and the other degradates using the RTX-200 column are shown in Appendix VI. Chromatography of a typical soil sample from study 92147 is also shown in Appendix VI.

H. **TIME REQUIRED FOR ANALYSIS**

The extraction of eight soil samples and the chromatography to develop the daily standard curve and run the eight samples and four day spikes and control can be done...
in 24 hours.

J. MODIFICATION OR POTENTIAL PROBLEMS

None.

K. CALCULATIONS

The peak areas corresponding to the eight compounds (PCB, HCB, PCP, PCNB, PCA, PCTA, TCTASOO, and PCTASO) in the standards were obtained from the chromatograms and regressed versus the concentration of the compounds in the standards. Statistics were generated on a Swan Corporation 386/33 computer using an Axum program capable of performing quadratic regression (second order polynomial regression) on the peak areas versus their corresponding concentrations to generate standard curves. The following quadratic equation was used:

$$\text{Peak Area} = b_0 + b_1 \cdot (\mu g/ml \text{ of standard}) + b_2 \cdot (\mu g/ml \text{ of standard})^2$$

In a few cases, peaks were found in the control samples. If required, a corrected peak area value was determined using the following formula:

$$\text{Peak area in sample corrected} = \text{Peak area in sample} - \text{Peak area in control}$$

The corrected peak area of each sample was used to calculate the amount in $\mu g/ml$ of each compound found in the samples analyzed relative to the generated standard curves. The square of the correlation coefficient ($R^2$) was used to evaluate the fit of the curve. The $\mu g/ml$ compound found value was then multiplied by the final volume of the sample to yield the $\mu g$ compound found.

$$\text{\mu g compound found} = [\mu g/ml \text{ compound found}] \times [\text{final volume (ml)}]$$

In fortified method spikes, the $\mu g$ compound found values were converted to ppm
compound found values by dividing by the sample weights. The ppm compound found values were then divided by ppm compounds added to obtain the percent recoveries.

If the average percent recovery for the two spiked samples of the set was below 100%, the amount of compound found in the sample was divided by the average recovery of the spikes to give the corrected value. No correction was made for average recoveries above 100%.

\[ \mu g \text{ compound found corrected} = \mu g \text{ compound found} / \text{average spike recovery} \]

In field samples, the ppm compound found was calculated using the \( \mu g \) compound found corrected for percent recovery divided by sample weight.

\[ \% \text{ moisture} = (\text{wet weight} - \text{dry weight} / \text{wet weight}) \times 100 \]

The average \% moisture for 2 aliquots was used to determine the \% soil moisture by the following equation:

\[ \text{ppm compound found} = \text{ppm compound found uncorrected} / \left[ \frac{100 - \% \text{ soil moisture}}{100} \right] \]
Figure I. Structures and chemical names of PCNB and other analytes.
Pentachlorothioanisole sulfoxide
(PCTASO)

Pentachlorothioanisole sulfone
(PCTASOO)

2,3,4,5-Tetrachlorothioanisole sulfone
(TCTASOO)

Figure I. (Continued)
Figure II. PCNB and Metabolites Analysis Method Flowchart
APPENDIX I

MSDS Sheets
Material Safety Data Sheet

UNIROYAL CHEMICAL
Uniroyal Chemical Company, Inc. UNIROYAL Emergency Phone: (203) 723-3570
World Headquarters CHEMTRAC Transportation Emergency Phone: 1-800-424-E
Middlebury, CT 06749 SAFETY DATA INFORMATION: (203) 573-3303
MSDS No. A390001 Date Issued: 10/15/85
UNIROYAL

NOTE TO END-USERS: This MSDS is being provided to all interested persons in accordance with federal and state right-to-know laws. Precautionary Statements, Statements of Practical Treatments, Directions for Use of this product by end-users are contained on the product label and must be followed at all times.

IDENTIFICATION
Trade Name: TERRACLOR® TECHNICAL
Chemical Name: Pentachloronitrobenzene
Inerts:
Common Name: PCNB
CAS Number: 82-66-8
Chemical Family: Halogenated Nitrobenzene 99%

SPECIAL REGULATORY HAZARDS
Ingredient CAS No. Exposure Limit OSHA (1910.1200) EEC*
PCNB 82-66-8 0.5 mg/m³, TWA Sensitizer Sensitize
(ACGIH) Carcinogen Harmful
Possible risk
Irreversible eff

Hazard assessment based on available data.
Transportation: DOT/ICAO/IATA Not Regulated
IMO Hazard Class: 9, Miscellaneous; ID No.: UN3077 Marine Pollutant

PHYSICAL DATA
Appearance and Odor: Light yellow to cream, crystalline solid; musty odor.
Solubility: Insoluble in water; soluble in organic solvents
Melting Point: 143°C (290°F)
Boiling Point: NA
Other Data: Bulk Density: 72 lbs/ft.³

FIRE AND EXPLOSION HAZARD DATA
Flash Point: ND Autoignition Temperature: ND
Extinguishing Media: Water spray, dry chemical.
Flammable Limits: ND
Special Fire Fighting Procedures: Protect against inhalation of combustion products. Contain run-off.

Unusual Hazards: None identified.

REACTIVITY DATA
Stability: Stable at ambient temperatures and pressures.
Incompatibility: Hydrolyzes with strong acids and alkalis.
Decomposition Products: May emit oxides of nitrogen, phosgene and hydrogen chloride under burning condition.

NA = Not Applicable
ND = Not Determined
* European Economic Community

Uniroyal makes no representation or warranty with respect to the information in this Material Safety Data Sheet. The information is however, as of date provided, true and accurate to the best of Uniroyal's knowledge. This list of information is not intended to be all inclusive. Actual conditions of use and handling may require considerations of information other than, or in addition to, that which is provided herein.

Page 35 of 166
SPECIAL PROTECTION INFORMATION

Engineering Controls: Sufficient ventilation to minimize dust exposure.

Personal Protection Equipment: Avoid all personal contact. Observe good personal hygiene. Chemical resistant gloves, protective clothing and eye protection should be worn when handling. Launder clothing before reuse. In the absence of adequate ventilation, use NIOSH-certified pesticide cartridge respirator.

NOTE TO END-USERS: The employee protection recommendations on this MSDS may differ from those on the product label. For normal use of this product, always refer to the personal protective equipment requirements on the product label.

STORAGE, SPILLS AND DISPOSAL INFORMATION

Storage: Store in a dry location.

Spills: Vacuum up to avoid creating dust. Transfer into secure containers for proper disposal. Use personal protective equipment as outlined above. Reportable Quantity: 100 lbs. (PCNB)

Disposal: Pesticide wastes are toxic. Improper disposal of excess pesticide, spray mixture, or rinseate is a violation of Federal Law. If these wastes cannot be disposed of by use according to label instructions, contact your State Pesticide or Environmental Control Agency, or the Hazardous Waste representative at the nearest EPA Regional Office for guidance.

Environmental Information: This pesticide is toxic to fish and aquatic organisms. Do not contaminate water when disposing of equipment washwaters. Do not discharge effluent containing this product into lakes, streams, ponds, estuaries, oceans, or public waters unless this product is specifically identified and addressed in an NPDES permit. Do not discharge effluent containing this product into sewer systems without previously notifying the sewage treatment plant authority. For guidance, contact your State Water Board or Regional Office of the EPA. Refer to EPA/OSWA Regulation 40 CFR 261.33(f) U185.

TERRACLOR TECHNICAL

TERRACLOR TECHNICAL BLUERIGG STURGEON: 96hr LC50 = 0.1 ppm
Rainbow Trout: 96hr LC50 = 0.3 ppm
Daphnia Magna: 96hr LC50 = 0.77 ppm
Fathead Minnow: Early Life Stage: 24-54 ug/l
Shoecreek Minnow: 96hr LC50 = 1.5 ppm

These data indicateTerraclor Technical to be very toxic to aquatic species and practically non-toxic to avian and other species.

HEALTH RELATED DATA

SPECIFIC HAZARDS: Slightly toxic by oral exposure. Repeated minimal contact with skin may cause sensitization. Tests in animals indicate PCNB to be an experimental animal carcinogen.

Primary Route(s) of Entry: Inhalation, skin absorption.

First Aid Procedures:

IF IN EYES: Immediately flush eyes with plenty of water and get medical treatment.

IF SWALLOWED: Call a physician or Poison Control Center immediately. Drink 1 or 2 glasses of water and induce vomiting by touching back of throat with finger. Do not induce vomiting or give anything by mouth to an unconscious person.

IF INHALED: See a physician if abnormal reaction occurs.

IF ON SKIN: Wash thoroughly with soap and water.

TOXICOLOGY INFORMATION:

Oral toxicity: LD50 (rats) - 5.0 g/kg
Dermal toxicity: LD50 (rabbits) - > 5.0 g/kg
Irritation: eye (rabbits) - slight
skin (rabbits) - negative
Sensitization: skin (guinea pigs) - sensitizer positive based on human patch testing

Chronic: A two year feeding study of PCNB in mice at dietary concentrations of 2500 and 5000 ppm did not show evidence of an increase in tumors.

A two year feeding study of PCNB in rats at dietary concentrations of 20, 3000 and 6000 ppm showed an increased incidence of thyroid follicular cell tumors. A subsequent mechanism study demonstrated that tumor formation was the result of altered thyroid hormone homeostasis, which has a threshold of 20 ppm (1 mg/kg/day). No teratogenic effects were seen in rat and rabbit teratology studies.

SARA TITLE III (40 CFR 372)
SECTION 313 TOXIC CHEMICALS NOTIFICATION

TOXIC CHEMICAL: pentachloronitrobenzene

CAS %: 82-08-8
% (BY. WT): 99.0%

TERRACLOR® TECHNICAL
SAMPLE FOR RESEARCH AND DEVELOPMENT ONLY
MUST ONLY BE HANDLED BY TECHNICALLY QUALIFIED PERSONS

Date:

MATERIAL SAFETY DATA SHEET

Trade Name/Code: PCAA, P-2 CAS No.:

Chemical Name: 2,3,4,5,6-Pentachloroaniline

PRECAUTION

The physical, chemical, and health hazards of this compound have not been fully investigated. It should be used and handled as though it is hazardous.

SPECIAL PROTECTION INFORMATION

Use adequate ventilation to prevent exposure to airborne dust, fume or vapor. Use good workplace practices and appropriate personal protective equipment to prevent exposure by inhalation, ingestion, absorption through skin and eye contact. Use NIOSH approved respiratory equipment as appropriate.

STORAGE, SPILLS AND DISPOSAL

Storage: Store away from sources of direct heat in a dry area. Keep containers closed.

Spills: Vacuum up, if solid. Absorb on inert material, if liquid. Transfer into secure containers for proper disposal. Do not flush to sewer.

Disposal: Disposal should be in accordance with applicable regulations for laboratory waste.

FIRST AID

Eye Contact: Flush with water for 15 minutes. Get medical attention.

Skin Contact: Wash with soap and water.

Ingestion: Use gastric lavage to empty stomach.

Inhalation: Move to fresh air. Get medical attention.

UNIROYAL Emergency Phone (203) 723-3670
SAFETY DATA Information (203) 573-3303

Uniroyal makes no representation or warranty with respect to the information in this Material Safety Data Sheet. The information is however, as of this date provided, true and accurate to the best of Uniroyal's knowledge. This list of information is not intended to be all inclusive. Actual conditions of use and handling may require considerations of information other than, or in addition to, that which is provided herein.
Material Safety Data Sheet

Product #: 13132-6
CAS #: 84-8-3
MF: C6H5C15

Synonyms
PCF * PENTACHLOROBENZENE * QCB * RCRA WASTE NUMBER U133 *

Toxicity Hazards

TECS NO.: 0A66-0000G
BENZENE, PENTACHLORO-

Toxicity Data

ORL-RAT LD50: 1030 MG/KG
ORL-MUS LD50: 1175 MG/KG

EPA-TSCA CHEMICAL INVENTORY

FINAL RULE FERAC

472-249920-82

WHMIS ANALYTICAL METHODS: SEE POLYCHLOROBENZENES:

NTP CARCINOGENESIS STUDIES TEST COMPLETED (POST PEEV REVIEW), JANUARY 1990

TARGET ORGAN DATA

BEHAVIORAL (GENERAL ANESTHETIC)

SPECIFIC DEVELOPMENTAL ABNORMALITIES (MUSCULOSKELETAL SYSTEM)

ONLY SELECTED REGISTRY OF TOXIC EFFECTS OF CHEMICAL SUBSTANCES (RTCS) DATA IS PRESENTED HERE. SEE ACTUAL ENTRY IN RTCS FOR COMPLETE INFORMATION

Health Hazard Data

CUT EFFECTS

HARMFUL IF SWALLOWED
MAY BE HARMFUL IF INHALED
MAY BE HARMFUL IF ABSORBED THROUGH THE SKIN

CAUSES EYES AND SKIN IRRITATION
MATERIAL IS IRRITATING TO MUCOUS MEMBRANES AND UPPER RESPIRATORY TRACT

TARGET ORGAN(S):
LIVER, KIDNEYS
BLOOD, THYROID

FIRST AID

IN CASE OF CONTACT, IMMEDIATELY FLUSH EYES WITH COPIOUS AMOUNTS OF WATER FOR AT LEAST 15 MINUTES
IN CASE OF CONTACT, IMMEDIATELY WASH SKIN WITH SOAP AND COPIOUS AMOUNTS OF WATER
IF INHALED, REMOVE TO FRESH AIR
IF NOT BREATHING GIVE ARTIFICIAL RESPIRATION
IF BREATHING IS DIFFICULT, GIVE OXYGEN
CALL A PHYSICIAN

CONTINUED ON NEXT PAGE
PRODUCT #: L3132-5  NAME: PENTACHLOROBENZENE, 98%
CAS #: 608-93-9  MF: C12H5Cl3

---------------------------------------- HEALTH HAZARD DATA ----------------------------------------
DISCARD CONTAMINATED CLOTHING AND SHOES.

---------------------------------------- PHYSICAL DATA ----------------------------------------
BOILING PT: 275°C TO 277°C
MELTING PT: 84°C TO 87°C
SPECIFIC GRAVITY: 1.609

APPEARANCE AND ODOR
OFF-WHITE POWDER WITH CHUNKS

---------------------------------------- FIRE AND EXPLOSION HAZARD DATA ----------------------------------------
TINGUISHING MEDIA
WATER SPRAY
CARBON DIOXIDE, DRY CHEMICAL POWDER, ALCOHOL OR POLYMER FOAM.

SPECIAL FIREFIGHTING PROCEDURES
WEAR SELF-CONTAINED BREATHING APPARATUS AND PROTECTIVE CLOTHING TO PREVENT CONTACT WITH SKIN AND EYES.

AVOID FIRE AND EXPLOSIONS HAZARDS
LIMIT TOXIC FUMES UNDER FIRE CONDITIONS.

---------------------------------------- REACTIVITY DATA ----------------------------------------
COMPATIBILITIES
STRENGTH OXIDIZING AGENTS
Hazardous Combustion Or Decomposition Products
TOXIC FUMES CF:
CARBON MONOXIDE, CARBON DIOXIDE
HYDROGEN CHLORIDE GAS

---------------------------------------- SPILL OR LEAK PROCEDURES ----------------------------------------
STEPS TO BE TAKEN IF MATERIAL IS RELEASED OR SPILLED
WEAR RESPIRATOR, CHEMICAL SAFETY GOGGLES, RUBBER BOOTS AND HEAVY RUBBER GLOVES.
SWEEP UP, PLACE IN A BAG AND HOLD FOR WASTE DISPOSAL.
AVOID Raising DUST.
VENTILATE AREA AND WASH SPILL SITE AFTER MATERIAL PICKUP IS COMPLETE.

SPILL DISPOSAL METHOD
DISSOLVE OR MIX THE MATERIAL WITH A COMBUSTIBLE SOLVENT AND BURN IN A CHEMICAL INCINERATOR EQUIPPED WITH AN AFTERBURNER AND SCRUBBER.
OBSERVE ALL FEDERAL, STATE, AND LOCAL LAWS.

--- PRECAUTIONS TO BE TAKEN IN HANDLING AND STORAGE ---
WEAR APPROPRIATE NIOSH/MSHA-APPROVED RESPIRATOR, CHEMICAL-RESISTANT GLOVES, SAFETY GOGGLES, OTHER PROTECTIVE CLOTHING.

CONTINUED ON NEXT PAGE.
PRODUCT #: 13132-6
CAS #: 603-93-5
    NAME: PENTACHLOROBENZENE, 98%

--- PRECAUTIONS TO BE TAKEN IN HANDLING AND STORAGE ---

SAFETY SHOWER AND EYE BATH.
MECHANICAL EXHAUST REQUIRED.
DO NOT BREATHE DUST.
AVOID CONTACT WITH EYES, SKIN AND CLOTHING.
WASH THOROUGHLY AFTER HANDLING.
IRRITANT.
HARMFUL SOLID.
STORE IN A COOL DRY PLACE.

THE ABOVE INFORMATION IS BELIEVED TO BE CORRECT BUT DOES NOT PURPORT TO BE
A COMPLETE AND SHALL BE USED ONLY AS A GUIDE. ALDRICH SHALL NOT BE HELD
ABLE OR ANY LIABILITY RESULTING FROM HANDLING OR CONTACT WITH THE
PRODUCT. SEE REVERSE SIDE OF INVOICE OR PACKING SLIP FOR ADDITIONAL
ERMS AND CONDITIONS OF SALE.

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Date: NOVEMBER 19, 1992

MATERIAL SAFETY DATA SHEET

Trade Name/Code: 2,3,4,5,6-PCTA-P-05
CAS No.:

Chemical Name: 2,3,4,5,6-Pentachlorothioanisole

PRECAUTION

The physical, chemical, and health hazards of this compound have
not been fully investigated. It should be used and handled as
though it is hazardous.

SPECIAL PROTECTION INFORMATION

Use adequate ventilation to prevent exposure to airborne dust,
fume or vapor. Use good workplace practices and appropriate
personal protective equipment to prevent exposure by inhalation,
ingestion, absorption through skin and eye contact. Use NIOSH
approved respiratory equipment as appropriate.

STORAGE, SPILLS AND DISPOSAL

Storage: Store away from sources of direct heat in a dry area.
Keep containers closed.

Spills: Vacuum up, if solid. Absorb on inert material, if
liquid. Transfer into secure containers for proper
disposal. Do not flush to sewer.

Disposal: Disposal should be in accordance with applicable
regulations for laboratory waste.

FIRST AID

Eye Contact: Flush with water for 15 minutes. Get medical
attention.

Skin Contact: Wash with soap and water.
Ingestion: Use gastric lavage to empty stomach.
Inhalation: Move to fresh air. Get medical attention.

UNIROYAL Emergency Phone (203) 723-3670
SAFETY DATA Information (203) 573-3303
ATTN: SAFETY DIRECTOR
UNITROYAL INC
OXFORD HG
R/D CENTER
MIDDLEBURY CT 06749
AL ORISCOLL/ MAIL CODE 1/2A

DATE: 07/2
CUST#: 483605
PO#: 3352-11-9433

MATERIAL SAFETY DATA SHEET

PRODUCT #: 17105-0
CAS #: 118-74-1
MF#: C6CL6

SYNONYMS
AMATIN * ANTICARIOSE * BUNT-CURE * BUNT-NO-MORE * CEKU C.B. * CO-OP
HEXA * ESACLOROBENZENE (ITALIAN) * GRANOX NM * HCB * HEXA C.B. *
HEXACHLOROBENZENE * HEXACHLOROBENZENE (Dlotte) *
JULIN'S CARBONIC/CHLORIDE * NO BUNT * NO BUNT 40 * NO BUNT 80 * NO
BUNT LIQUID * PENTACHLOROPHENYL CHLORIDE * PERCHLOROBENZENE * PHENYL
PERCHLORYL * SANOCIDE * SHUT-60 * TCRA WASTE NUMBER U1277 *
SAATBEIZUNGZEIT(german) * SANOCID * SNIJCIETOX * UN-2729 (Dotte) *

TOxicity Hazards

RTC#S NO: DA2975000;
BENZENE, HEXACHLORO-

TOxicity DATA
UN-RAT LD50L: 1200 MG/KG
ORL-RAT LD50: 110 GM/KG
IHL-RAT LC50: 3000 MG/M3
ORL-MUS LD50: 40 GM/KG
SCU-MUS LD50: 10 GM/KG
ORL-CAT LD50: 1700 MG/KG
IHL-CAT LD50: 1600 MG/M3
ORL-RBT LD50: 2600 MG/KG
ORL-SPG LD50: 3 MG/KG
ORL-MAM LD50: 1047 MG/KG

REVIEWS, STANDARDS, AND REGULATIONS
IARC CANCER REVIEW: ANIMAL SUFFICIENT EVIDENCE IMMUTATION 20: 155, 79
IARC CANCER REVIEW: HUMAN INADEQUATE EVIDENCE IMMUTATION 20: 721, 97
NOES 1.98 HZD AL 7.59; NO 10; NOS 12; TNE 1038; TFE 26
EPA GENETOX PROGRAM 1988: POSITIVE: CARCINOGENICITY-HOUSE/RAT
EPA GENETOX PROGRAM 1988: NEGATIVE: RODENT DOMINANT LEATHAL
EPA TSCA CHEMICAL INVENTORY, JUNE 1990
ON EPA ITRIS DATABASE
NTP FIFTH ANNUAL REPORT ON CARCINOGENS, 1989: ANTICIPATED TO BE
CARCINOGEN
TARGET ORGAN DATA
BEHAVIORAL (SOMNOLENCE)
LIVER (TUMORS)

CONTINUED ON NEXT PAGE
PRODUCT #: 17105-0
CAS #: 118-74-1
NAME: HEXACHLOROBENZENE, 99%
MF: C6C16

----------------------------------------------------------------- TOXICITY HAZARDS
-----------------------------------------------------------------
ENDOCRINE (THYROID-TUMORS)
SPECIFIC DEVELOPMENTAL ABNORMALITIES (CRANIOFACIAL)
SPECIFIC DEVELOPMENTAL ABNORMALITIES (MUSCULOSKELETAL SYSTEM)
SPECIFIC DEVELOPMENTAL ABNORMALITIES (UGENITAL SYSTEM)
EFFECTS ON NEWBORN (LIVE BIRTH INDEX)
EFFECTS ON NEWBORN (VIABILITY INDEX)
EFFECTS ON NEWBORN (HEALTH OR LACTATION INDEX)
EFFECTS ON NEWBORN (GROWTH STATISTICS)
EFFECTS ON NEWBORN (BIOCHEMICAL AND METABOLIC)
TUMORIGENIC (CARCINOGENIC BY RTECS CRITERIA)
TEUMORIGENIC (NEOPLASTIC BY RTECS CRITERIA)
BIOCHEMICAL EFFECTS (PORPHYRIN INCLUDING BILE PIGMENTS)

ONLY SELECTED REGISTRY OF TOXIC EFFECTS OF CHEMICAL SUBSTANCES (RTECS) DATA IS PRESENTED HERE. SEE ACTUAL ENTRY IN RTECS FOR COMPLETE INFORMATION.

---------------------------------------------------------------- HEALTH HAZARD DATA
----------------------------------------------------------------

ACUTE EFFECTS
HARMFUL IF SWALLOWED, INHALED, OR ABSORBED THROUGH SKIN.
CAUSES EYE AND SKIN IRRITATION.
MATERIAL IS IRRITATING TO MUCOUS MEMBRANES AND UPPER RESPIRATORY TRACT.
CAUSES PHOTOSensitivity. EXPOSURE TO LIGHT CAN RESULT IN ALLERGIC REACTIONS RESULTING IN DERMATOLOGIC LESIONS, WHICH CAN VARY FROM SUNBURNLIKE RESPONSES TO EDENATOUS, VESICULATED LESIONS OR BULLAe.
CHRONIC EFFECTS
CARCINOGEN.
HAY ALTER GENETIC MATERIAL.
TARGET ORGAN(S):
LIVER
FIRST AID
IN CASE OF CONTACT, IMMEDIATELY FLUSH EYES OR SKIN WITH COPIOUS AMOUNTS OF WATER FOR AT LEAST 15 MINUTES WHILE REMOVING CONTAMINATED CLOTHING AND SHOES.
IF INHALED, REMOVE TO FRESH AIR. IF NOT BREATHING GIVE ARTIFICIAL RESPIRATION. IF BREATHING IS DIFFICULT, GIVE OXYGEN.
IF SWALLOWED, WASH OUT MOUTH WITH WATER PROVIDED PERSON IS CONSCIOUS.
CALL A PHYSICIAN.
DISCARD CONTAMINATED CLOTHING AND SHOES.

BOILING PT: 323 C TO 326 C

CONTINUED ON NEXT PAGE
PRODUCT #: 17105-0  
CAS #: 266-74-1  
NAME: HEXACHLOROBENZENE, 99%  
HF #: C6C6L6

--- PHYSICAL DATA ---
HEATING PT: 227 °C TO 229 °C  
APPEARANCE AND ODOR: WHITE POWDER  
FIRE AND EXPLOSION HAZARD DATA ---
EXTINGUISHING MEDIA: WATER SPRAY  
CARBON DIOXIDE, DRY CHEMICAL POWDER OR APPROPRIATE FOAM  
SPECIAL FIREFIGHTING PROCEDURES: WEAR SELF-CONTAINED BREATHING APPARATUS AND PROTECTIVE CLOTHING TO PREVENT CONTACT WITH SKIN AND EYES  
UNUSUAL FIRE- AND EXPLOSION HAZARDS: EMITS TOXIC FUMES UNDER FIRE CONDITIONS.

--- INCOMPATIBILITIES ---
STRONG OXIDIZING AGENTS  
HAZARDOUS COMBUSTION OR DECOMPOSITION PRODUCTS: TOXIC FUMES OF: CARBON MONOXIDE, CARBON DIOXIDE, HYDROGEN CHLORIDE GAS

--- SPILL OR LEAK PROCEDURES ---
STEPS TO BE TAKEN IF MATERIAL IS RELEASED OR SPILLED: EVACUATE AREA  
WEAR SELF-CONTAINED BREATHING APPARATUS, RUBBER BOOTS AND HEAVY RUBBER GLOVES  
WEAR DISPOSABLE COVERALLS AND DISCARD THEM AFTER USE  
SHEEP UP: PLACE IN A BAG AND HOLD FOR WASTE DISPOSAL  
VENTILATE AREA AND WASH SPILL SITE AFTER MATERIAL PICKUP IS COMPLETE.

--- WASTE DISPOSAL METH " ---
DISSOLVE OR MIX THE MATERIAL WITH A COMBUSTIBLE SOLVENT AND BURN IN A CHEMICAL INCINERATOR EQUIPPED WITH AN AFTERBURNER AND SCRUBBER  
OBSERVE ALL FEDERAL, STATE AND LOCAL ENVIRONMENTAL REGULATIONS.

--- PRECAUTIONS TO BE TAKEN IN HANDLING AND STORAGE ---
WEAR APPROPRIATE NIOSH/OSHA-APPROVED RESPIRATOR, CHEMICAL-RESISTANT

CONTINUED ON NEXT PAGE
PRODUCT #: 17105-0
NAME: HEXACHLOROBENZENE, 99%
CAS #: 118-74-1
MF: C6Cl6

--- PRECAUTIONS TO BE TAKEN IN HANDLING AND STORAGE ---

GLOVES, SAFETY GOGGLES, OTHER PROTECTIVE CLOTHING.
SAFETY SHOWER AND EYE BATH.
USE ONLY IN A CHEMICAL FUME HOOD.
DO NOT BREATHE DUST.
AVOID ALL CONTACT.
WASH THOROUGHLY AFTER HANDLING.
CARCINOGEN.
IRRITANT.
PHOTOSENSITIZER.
MUTAGEN.
HARMFUL SOLID.
KEEP TIGHTLY CLOSED.
STORE IN A COOL, DRY PLACE.

REGULATORY INFORMATION
THIS PRODUCT IS SUBJECT TO SARA SECTION 313 REPORTING REQUIREMENTS.

THE ABOVE INFORMATION IS BELIEVED TO BE CORRECT BUT DOES NOT PURPORT TO BE
ALL INCLUSIVE AND SHALL BE USED ONLY AS A GUIDE. ALDRICH SHALL NOT BE HELD
ABLE FOR ANY DAMAGE RESULTING FROM HANDLING OR FROM CONTACT WITH THE
OVE PRODUCT. SEE REVERSE SIDE OF INVOICE OR PACKING SLIP FOR ADDITIONAL
TERMS AND CONDITIONS OF SALE.

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Date: 7/7/1995

MATERIAL SAFETY DATA SHEET

Trade Name/Code: PCP- P-38
CAS No.: 
Chemical Name: Pentachlorophenol

PRECAUTION

The physical, chemical, and health hazards of this compound have not been fully investigated. It should be used and handled as though it is hazardous.

SPECIAL PROTECTION INFORMATION

Use adequate ventilation to prevent exposure to airborne dust, fume or vapor. Use good workplace practices and appropriate personal protective equipment to prevent exposure by inhalation, ingestion, absorption through skin and eye contact. Use NIOSH approved respiratory equipment as appropriate.

STORAGE, SPILLS AND DISPOSAL

Storage: Store away from sources of direct heat in a dry area. Keep containers closed.

Spills: Vacuum up, if solid. Absorb on inert material, if liquid. Transfer into secure containers for proper disposal. Do not flush to sewer.

Disposal: Disposal should be in accordance with applicable regulations for laboratory waste.

FIRST AID

Eye Contact: Flush with water for 15 minutes. Get medical attention.
Skin Contact: Wash with soap and water.
Ingestion: Use gastric lavage to empty stomach.
Inhalation: Move to fresh air. Get medical attention.

UNIROYAL Emergency Phone (203) 723-3670
SAFETY DATA Information (203) 573-3303

Uniroyal makes no representation or warranty with respect to the information in this Material Safety Data Sheet. The information is however, as of this date provided, true and accurate to the best of Uniroyal’s knowledge. This list of information is not intended to be all inclusive. Actual conditions of use and handling may require considerations of information other than, or in addition to, that which is provided herein.
SAMPLE FOR RESEARCH AND DEVELOPMENT ONLY
MUST ONLY BE HANDLED BY TECHNICALLY QUALIFIED PERSONS

Date: NOVEMBER 19, 1992

MATERIAL SAFETY DATA SHEET

Trade Name/Code: PCTASO-P-45
Chemical Name: Pentachlorothioanisole sulfoxide

CAS No.: 

PRECAUTION

The physical, chemical, and health hazards of this compound have not been fully investigated. It should be used and handled as though it is hazardous.

SPECIAL PROTECTION INFORMATION

Use adequate ventilation to prevent exposure to airborne dust, fume or vapor. Use good workplace practices and appropriate personal protective equipment to prevent exposure by inhalation, ingestion, absorption through skin and eye contact. Use NIOSH approved respiratory equipment as appropriate.

STORAGE, SPILLS AND DISPOSAL

Storage: Store away from sources of direct heat in a dry area. Keep containers closed.

Spills: Vacuum up, if solid. Absorb on inert material, if liquid. Transfer into secure containers for proper disposal. Do not flush to sewer.

Disposal: Disposal should be in accordance with applicable regulations for laboratory waste.

FIRST AID

Eye Contact: Flush with water for 15 minutes. Get medical attention.

Skin Contact: Wash with soap and water.

Ingestion: Use gastric lavage to empty stomach.

Inhalation: Move to fresh air. Get medical attention.

UNIROYAL Emergency Phone (203) 723-3670
SAFETY DATA Information (203) 573-3303
SAMPLE FOR RESEARCH AND DEVELOPMENT ONLY
MUST ONLY BE HANDLED BY TECHNICALLY QUALIFIED PERSONS

Date: NOVEMBER 19, 1992

MATERIAL SAFETY DATA SHEET

Trade Name/Code: 2,3,4,5-TCTAS00-P-55 CAS No.: 

Chemical Name: 2,3,4,5-Tetrachlorothioanisole sulfone 

PRECAUTION

The physical, chemical, and health hazards of this compound have not been fully investigated. It should be used and handled as though it is hazardous. 

SPECIAL PROTECTION INFORMATION

Use adequate ventilation to prevent exposure to airborne dust, fume or vapor. Use good workplace practices and appropriate personal protective equipment to prevent exposure by inhalation, ingestion, absorption through skin and eye contact. Use NIOSH approved respiratory equipment as appropriate.

STORAGE, SPILLS AND DISPOSAL

Storage: Store away from sources of direct heat in a dry area. Keep containers closed.

Spills: Vacuum up, if solid. Absorb on inert material, if liquid. Transfer into secure containers for proper disposal. Do not flush to sewer.

Disposal: Disposal should be in accordance with applicable regulations for laboratory waste.

FIRST AID

Eye Contact: Flush with water for 15 minutes. Get medical attention.

Skin Contact: Wash with soap and water.

Ingestion: Use gastric lavage to empty stomach.

Inhalation: Move to fresh air. Get medical attention.

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