



CHEMICALS • EQUIPMENT • HEALTH PRODUCTS

FYI-0794-1031

900 FIRST AVENUE, P.O. BOX C, KING OF PRUSSIA, PENNSYLVANIA 19406 • (215) 265-3200



FYI-94-001031
INIT 07/14/94

#022484(2)

February 13, 1984

CBI Available #20-8480246-1

Mr. Martin Greif
Executive Secretary
TSCA Interagency Testing Committee
Environmental Protection Agency
401 M Street, NW
Washington, DC 20460



84948000131

Dear Mr. Greif:

This letter and attachments are in response to the Federal Register Notice (FR48: 51519-51521) dated November 9, 1983. At this time we are submitting information on the following Pennwalt products:

CAS No.

Chemical Name

<i>1R-419</i> 100-37-8	2-(diethylamino)ethanol
<i>1R-417A</i> 95-31-8	N-tert-butyl-2-benzothiazole sulfenamide
<i>1R-417B</i> 95-33-0	N-cyclohexyl-2-benzothiazole sulfenamide
<i>1R-432</i> 120-78-5	2,2-dithiohisbenzothiazole
<i>1R-406A</i> 80-43-3	cumene peroxide
<i>1R-406B</i> 110-05-4	di-tert-butyl peroxide

A small portion of the information on each product is being submitted as Confidential Business Information (CBI). Accordingly, this information is attached separately in the envelope marked "TSCA-CBI" and should be treated as confidential in accordance with established procedures.

We appreciate the opportunity to submit this information on Pennwalt products. If there are any questions regarding this submission, we will be pleased to respond.

Very truly yours,

John E. Hopkins /jm

John E. Hopkins
Director
Occupational Health & Safety

JEH/jm
Attachments

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N-tert-butyl-2-benzothiazolesulfenamide
(CAS: 95-31-8)

Product Literature

Attached are copies of a Technical Data Sheet and Material Safety Data Sheet for PENNAC® TBBS - Pennwalt's product name for n-tert-butyl-2-benzothiazolesulfenamide (TBBS).

Annual Production Data and Trends

Confidential Business Information (CBI)
See enclosed envelope marked "TSCA-CBI".

Production Worker Exposure

Pennwalt has no domestic in-plant exposure for TBBS since the material is imported already bagged for domestic sale.

Product Use Exposure

Pennwalt is not familiar with personnel exposure during use of this material in the rubber manufacturing process. This exposure information is probably best determined through representatives of the rubber manufacturing industry. Occasional exposure to this material will occur, however, when bags are accidentally broken in transit or in the warehouses.

TBBS is consumed by reaction mechanisms during normal processing in the manufacture of rubber. Therefore, human exposure to this material following the rubber manufacturing process is not anticipated.

Environmental Exposure

TBBS is unlikely to have any significant environmental impact because it is consumed through reaction mechanisms during its use in the rubber manufacturing process.

The most likely routes of entry to the environment are through spillage or breakage, which are not predictable, and residue in bags. The bag residue, if not consumed during disposal by incineration, would amount to less than 1000 lbs. per 200,000 lbs. of starting material per year, assuming that 4 oz. is left in each bag.

N-tert-butyl-2-benzothiazolesulfenamide

(CAS: 9-31-8)

Page 2



Toxicological Data

Pennwalt does not possess any internally generated toxicity data for TBBS. The acute oral data (LC₅₀ for rats is greater than 6.31 gm/kg) and acute dermal data (non-lethal to rabbits at 7.94 gm/kg) as shown on the attached MSDS suggest a relatively low order of acute toxicity.

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PENNVALTCHEMICALS • EQUIPMENT
HEALTH PRODUCTS

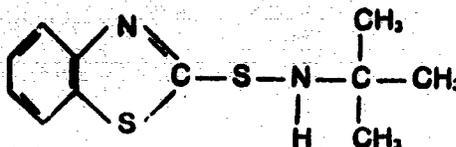
120-A North Main Street, Hudson, Ohio 44238 • (216) 850-4428

RUBBER ACCELERATORS

PENNAC TBS-O

00743

FORMULA



CHEMICAL NAME

N-tertiary-butyl-2-benzothiazole-sulfenamide (CAS No. : 95-31-8)

PROPERTIES

Molecular Weight 238.4
 Specific Gravity 1.28
 Oil treated to reduce dust in handling.

SPECIFICATIONS

Appearance off white
 Melting point 105° C min.
 Oil content 1.5 ± 0.5%
 Ash 0.5% max.
 Moisture 0.5% max.
 Insoluble in methanol 1.0% max.
 Fineness (thru 30 mesh) 99.5% min.

APPLICATIONS

Non staining accelerator for IR, SBR, IR, BR.

PACKAGING

25 kg. (55 lbs.) net weight
 Paper bags with PE laminated inner liner
 Palletized on wooden pallets.

SHIPPING

Freight Classification: Rubber Accelerators or
 Softeners NOIBN. Parcel post, air express, air
 freight allowed.

HANDLING

Material Safety Data Sheet available on request.

1/1/83



MATERIAL SAFETY DATA SHEET

"ESSENTIALLY SIMILAR" TO OSHA FORM 20
FORM 4040 (Rev. 9-80)

ADDRESS: Pennac Corporation

Three Parkway
Philadelphia, PA 19102

PRODUCT IDENTIFICATION

Pennac Product Name PENNAC TBBS - POWDER	Pennac Code No. 0640
Chemical Name and Molecular Formula 2-Benzothiazolesulfenamide, N-(1,1-dimethyl-ethyl)- C₁₁H₁₄N₂S₂	
Synonyms N-tert-Butyl-2-Benzothiazolesulfenamide	

Emergency Phone Number(s) Business: 215-587-7550 Other: 313-285-9200	
CAS No.(s) 95-31-8	Chemical Family Aryl Cyclic Sulfide Amide

HAZARDOUS INGREDIENTS

MATERIALS OR COMPONENTS	% w/w
N-tert-Butyl-2-Benzothiazolesulfenamide	93min.

HAZARD DATA (TLV, LD50, LC50, etc.)

See Toxicity Section.
OCCUPATIONAL HEALTH & SAFETY

REC'D JA 16 1984

READ BY _____ DATE _____
ANS BY _____ DATE _____

SHIPPING INFORMATION

Shipping Description Rubber Accelerators or Softeners, NOIBN	Packaging Multiwall paper bag - 50 lbs. net Fiber drum - 175 lbs. net
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PHYSICAL PROPERTIES

Boiling Point/Range °C _____ °F _____	Melting Point °C 104 °F _____	Freezing Point °C _____ °F _____	Molecular Weight (Calculated) 238.37
Specific Gravity (H ₂ O=1) 1.25-1.31 @ 25 / 25 °C	Vapor Pressure (mm Hg) @ _____ °C _____ °F	Vapor Density (Air=1)	
Solubility in H ₂ O negligible	% Volatiles by Volume 0.5 max.	Evaporation Rate <input type="checkbox"/> Ether = 1 <input type="checkbox"/> Water = 1 <input type="checkbox"/> Butylacetate = 1	
Appearance and Odor Light tan to buff	Other		

FLAMMABLE DATA

Flash Point °C _____ °F _____	Test Method Nonflammable	Flammable Limits Lower _____ % Upper _____ %	Auto-ignition Temperature/Fire Point °C _____ °F _____
EXTINGUISHING MEDIA <input type="checkbox"/> Water-spray <input type="checkbox"/> Water-fog <input type="checkbox"/> Water stream <input type="checkbox"/> CO ₂ <input type="checkbox"/> Dry chemical <input type="checkbox"/> Alcohol foam <input type="checkbox"/> Foam <input type="checkbox"/> Earth or sand			

SPECIAL FIRE FIGHTING PROCEDURES

Do not enter building Allow fire to burn Water: may cause frothing Do not use water

UNUSUAL FIRE AND EXPLOSION HAZARDS

Dust explosion hazard Sensitive to shock Contamination Temperature Other (specify): _____

STABILITY

STABILITY <input checked="" type="checkbox"/> Stable <input type="checkbox"/> Unstable	CONDITIONS CONTRIBUTING TO INSTABILITY <input type="checkbox"/> Thermal decomposition <input type="checkbox"/> Photo degradation <input type="checkbox"/> Polymerization <input type="checkbox"/> Contamination
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INCOMPATIBILITY - Avoid contact with:

Strong acids Strong alkalis Strong oxidizers Other (specify): _____

HAZARDOUS DECOMPOSITION PRODUCTS - THERMAL AND OTHER (list)

CONDITIONS TO AVOID

Heat Open flames Sparks Ignition sources Other (specify): _____

STEPS TO BE TAKEN IF MATERIAL IS RELEASED OR SPILLED

Flush with water Absorb with sand or inert material Neutralize Sweep or scoop up and remove Keep upwind. Evacuate enclosed spaces. Prevent spread or spill

WASTE DISPOSAL METHOD - Consult federal, state, or local authorities for proper disposal procedures.

NA - Not Applicable.

CONTINUED ON REVERSE SIDE

LD₅₀ is greater than 6.31 gm/kg (rats)

All rabbits survived applications of 7.94 gm/kg

Eyes: Slight irritation Inhalation (acute): Discomfort from "inert" dust

Derms, Substrates, etc.

Patch testing resulted in the conclusion that Pennac TBBS "was not a primary skin irritant, a fatiguing agent, or a sensitizing agent".

PERMISSIBLE EXPOSURE LIMIT (Specify if TLV/TWA or Ceiling (c))
ACGIH 19 OSHA 19 Other: Not established

IRRITATION
 Skin Severe Moderate
 Eye Severe Moderate Mild (transient)

CORROSIVITY
 Skin 4 hrs. (DOT) 24 hrs. (CPSC)
 Eye May cause blindness

SENSITIZATION
 Skin Respiratory Allergen **INHALATION EFFECTS**
 Narcotic effect Cyanosis Asphyxiant

LUNG EFFECTS (Specify):

OTHER (Specify):
 Repeated contact - skin defatter Other (Specify):

INGESTION
 Induce vomiting Do NOT induce vomiting Give plenty of water Get medical attention Other (specify):

DERMAL
 Flush with soap and water Get medical attention Contaminated clothing - remove & launder Contaminated shoes - destroy Other (specify):

EYE CONTACT
 Flush with plenty of water for at least 15 minutes Get medical attention Other (specify):

INHALATION
 Remove to fresh air If not breathing, give artificial respiration Give oxygen Get medical attention Other (specify):

VENTILATION REQUIREMENTS - Always maintain exposure below permissible exposure limits
 Consult an industrial hygienist or environmental health specialist Local exhaust Use with adequate ventilation Check for air contaminant and oxygen deficiency

Other (specify):

EYE
 Safety glasses Face shield Goggles
HAND (GLOVE TYPE)
 Polyvinyl chloride Neoprene Butyl rubber Polyvinyl alcohol Other (specify):
 Natural rubber Polyethylene

RESPIRATOR TYPE - Use only NIOSH / MESA approved equipment
 Self-contained Supplied air Can or cartridge gas or vapor Filter - dust Other (specify): **If not controlled by ventilation.**

OTHER PROTECTIVE EQUIPMENT
 Rubber boots Apron Other (specify):

PRECAUTIONARY LABELING
 Wash thoroughly after handling Do not get in eyes, Do not breathe dust Keep container closed Keep away from heat, sparks, and open flames Store in tightly closed containers

Do not store near combustibles Keep from contact with clothing and other combustible materials Empty container may contain hazardous residues Use explosion proof equipment Other (specify):

Other handling and storage conditions

Prepared by Christie B. Johnson **Date** 2/20/81 **Address** 3 Parkway, Philadelphia, PA 19102 **Phone** 215-587-7550

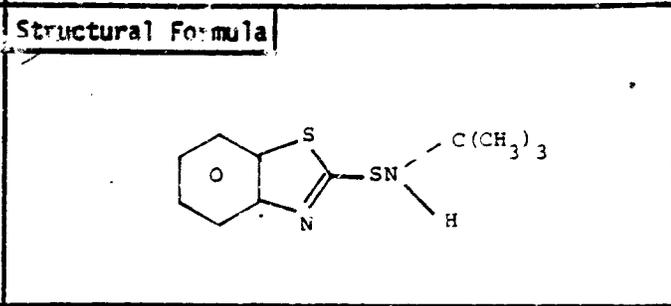
PLEASE NOTE ▶ "The above information is accurate to the best of our knowledge. However, since data, safety standards, and government regulations are subject to change and the conditions of handling and use, or misuse are beyond our control, Pennac MAKES NO WARRANTY, EITHER EXPRESS OR IMPLIED, WITH RESPECT TO THE COMPLETENESS OR CONTINUING ACCURACY OF THE INFORMATION CONTAINED HEREIN AND DISCLAIMS ALL LIABILITY FOR RELIANCE THEREON. User should satisfy himself that he has all current data relevant to his particular use."

EFFECTS INFORMATION PROFILE

ID No.	CHEMICAL NAME	SYNONYMS	CAS No.
35	2-Benzothiazolesulfenamide, N- (1,1 -dimethyl ethyl)		95-31-8

Description	Use

Melting point:
 Vapor pressure (B.P.):
 Specific gravity:
 Water solubility:
 Organic solubility:
 Log P oct/water: 1.85
 Empirical formula: $C_{11}H_{14}N_2S_2$



Biochemical Information

Reference	Nature of Info.	Page

Observations in Humans

Reference	Nature of Info.	Page

Environmental Information

Reference	Nature of Info.	Page

Toxicological Information

Reference	Nature of Info.	Page

Enclosures

Page
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CURRENT AWARENESS FILE

2-BENZOTHIAZOLESULFENAMIDE, N-tert-BUTYL-

CGNO. 5318

7908

C11-H14-W2-S

205.33

155 BN DSJ CSMX12121

N-tert-BUTYL-2-BENZOTHIAZOLESULFENAMIDE

LD50: 180 mg/kg

REPORTED IN EPA TSCA INVENTORY, 1980

ON-LINE-TOXICOLOGY DATA BANK-NLM, DECEMBER 1982

CSLNX NX#02241

NIOSH PROFILE (MERCAPTOBENZOTHIAZOLES), SRC, 3/78
EPA TSCA 8(a) PRELIMINARY ASSESSMENT INFORMATION PROPOSED RULE

FERZAC 45.13646.80

2-(Diethylamino)ethanol
(CAS: 100-37-8)

Contains No CBI

Product Literature

Attached is a copy of the Material Safety Data Sheet and Pennwalt sales bulletin for PENNADe 150 - Pennwalt's product name for diethylaminoethanol (DEAE).

Production Data and Trends

Confidential Business Information (CBI).
See enclosed envelope marked "TSCA-CBI".

Product Worker Exposure

Confidential Business Information (CBI).
See enclosed envelope marked "TSCA-CBI".

Product Use Exposure

There are many end uses for DEAE. Some of these uses include corrosion inhibitor, organic intermediate, curing agent, and emulsifying agent. Because of these multiple uses, it is difficult to estimate the end product human exposure. Pennwalt does not have the necessary information to make such an estimate.

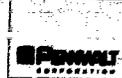
A portion of this information is classified as Confidential Business Information (CBI). See enclosed envelope marked "TSCA-CBI".

However, according to recent NIOSH Health Hazard Evaluation Reports^{1,2}, DEAE was monitored during periods of space humidification in two separate cases where it was used as a corrosion inhibitor for boiler water. Levels of DEAE were found

¹ Nicholas Fannick et al., Health Hazard Evaluation Report No. 83-020-1351: Johnson Museum Cornell University, Ithaca, New York, NIOSH, 1983.

² Kevin P. McManus et al., Health Hazard Evaluation Report No. 81-247-958: Boehringer Ingleheim, Ltd., Cincinnati, Ohio, NIOSH, 1981.

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to be at or below the limit of detection in air (0.04 mg/m³). This is well below the OSHA permissible exposure limit of 50 mg/m³. Varying amounts of DEAE salt deposits, however, were found on surfaces in these buildings.

Environmental Exposure

Losses of DEAE to the environment during production are minimized since waste material from this process is either recycled or contained for later contract disposal.

The single largest source of DEAE reaching the environment is likely to derive again from its use as a boiler water corrosion inhibitor. Nearly all of the DEAE in this use reenters the environment as DEAE or a salt of DEAE. The major portion of this exits the boiler as "blow down" where the DEAE-CO₂ reaction product is predominant.

Toxicological Data

Attached are copies of the following unpublished toxicology reports on DEAE:

1. Pharmacology Research report dated March 13, 1958, entitled "Sensitization Studies with Dimethylamino-Ethanol (DMAE) and with Diethylamino-Ethanol (DEAE)."
2. Pharmacology Research report dated August 1, 1977, entitled "Diethylaminoethanol #0129 (1) Eye Irritancy in Rabbits and (2) DOT Skin Corrosivity in Rabbits."
3. Scientific Associates report dated July 31, 1967, entitled "Final Report on Two-Year Chronic Feeding of Diethylaminoethanol to Albino Rats" (Study Number 101332).
4. Scientific Associates report dated December 30, 1966, entitled "Final Report on One-Year Chronic Feeding in Beagle Dogs of Diethylaminoethanol" (Study Number 101333). Only the first eleven pages of this report are available from the files.

The above chronic toxicology studies were sponsored by Pennwalt and the results were used in a Food Additive Petition to the U.S. Food and Drug Administration (FDA). The FDA granted an allowance for a concentration of DEAE up to 15 ppm in steam which comes in contact with food products, excluding milk and milk products.

The acute toxicology studies (also sponsored by Pennwalt) indicate the DEAE was noncorrosive and nonsensitizing to the skin when tested with rabbits and guinea pigs respectively. Results of eye irritancy testing with rabbits indicated that DEAE is corrosive.



MATERIAL SAFETY DATA SHEET

"ESSENTIALLY SIMILAR" TO OSHA FORM 20
Form 6040 (Rev. 6-81)

ADDRESS: **newark Corporation**
Thru Parkway
Philadelphia, PA 19102

Product Name: **PENNAD 150** Form Code No.: **0150**

Emergency Phone Number(s)
Business: **215/587-7550**
Other: **313/265-9200**

Chemical Name and Molecular Formula
Ethanol, 2-(diethylamino) C₆H₁₅NO

CAS No. (s)
100-37-8

Synonyms: **Diethylaminoethanol, 2-Hydroxytriethylamine, Diethylethanolamine**

Chemical Family
Alkyl Amine

MATERIALS OR COMPONENTS	% w/w	HAZARD DATA (TLV, LD50, LCS0, etc.)
Diethylaminoethanol	99.5 min.	See Toxicity Section

Drums: **Chemicals NOIBN.**
T/T: **Combustible Liquids NOS; Combustible Liquid; NA 1993; Combustible Placards, Diethylaminoethanol.**
T/C: **Combustible Liquid NOS; Combustible Liquid; NA 1993; Placarded Combustible; Diethylaminoethanol.**

Boiling Point/Range: **158-163.5 °C 316-326°F** Melting Point: **°C °F -56 °C -49°F** Molecular Weight (Calculated): **117.2**

Specific Gravity (H₂O=1): **0.88-0.89 @ 20/20 °C** Vapor Pressure (mm Hg): **1.4 @ 20 °C °F** Vapor Density (Air=1): **4.0**

Solubility in H₂O: **Complete** % Volatiles by Volume: **100** Evaporation Rate: Ether = 1 Water = 1 Butylacetate = 1

Appearance and Odor: **Water white, amine odor.** Other: _____

Flash Point: **°C 125 °F** Test Method: **T.C.C.** Flammable Limits: **Lower % Upper %** Autoignition Temperature/Fire Point: **°C °F**

EXTINGUISHING MEDIA
 Water-spray water-fog Water stream CO₂ Dry chemical Alcohol foam Foam Earth or sand

SPECIAL FIRE FIGHTING PROCEDURES
 Do not enter building Allow fire to burn Water may cause frothing Do not use water

UNUSUAL FIRE AND EXPLOSION HAZARDS
 Dust explosion hazard Sensitive to shock Contamination Temperature Other (specify): _____

STABILITY CONDITIONS CONTRIBUTING TO INSTABILITY
 Stable Unstable Thermal decomposition Photo degradation Polymerization Contamination

INCOMPATIBILITY - Avoid contact with
 Strong acids Strong alkalis Strong oxidizers Other (specify): _____

HAZARDOUS DECOMPOSITION PRODUCTS - THERMAL AND OTHER (list): _____

CONDITIONS TO AVOID
 Heat Open flames Sparks Ignition sources Other (specify): _____

STEPS TO BE TAKEN IF MATERIAL IS RELEASED OR SPILLED
 Flush with water Absorb with sand or inert material Neutralize Sweep or scoop up and remove Keep upwind. Evacuate enclosed spaces. Prevent spread of spill
 Dispose of immediately Other (specify): _____

*Small spills (less than one gallon) may be flushed away with water if permitted.
WASTE DISPOSAL METHOD - Consult federal, state, or local authorities for proper disposal procedures.

CONTINUED ON REVERSE SIDE
10/15/82

NA - Not Applicable.

Before using product, read and follow directions and precautions on product label and literature.

LD50 (mouse) 1300 mg/kg rat.

Dermal (acute) LD50: 1250 mg/kg rabbit.

Eye Corrosive, causes intense pain
Inhalation (acute) LC20 saturated vapor, 8H rat.

Chronic, Subchronic, etc.

PERMISSIBLE EXPOSURE LIMIT (Specify TLV/TWA or Ceiling (c))
ACGIH 19 81 TLV 10ppm OSHA 19 81 TWA 10ppm Other: Both designate "skin".

IRRITATION Skin Severe Moderate
 Eye Severe Moderate Mild (transient)

CORROSIVITY Skin 4 hrs. (DOT) 24 hrs. (CPSC)
 Eye May cause blindness

SENSITIZATION Skin Respiratory Allergen
INHALATION EFFECTS Narcotic effect Cyanosis Asphyxiant

LUNG EFFECTS (Specify):

OTHER (Specify):
 Repeated contact skin irritate Other (Specify):

INGESTION Induc. vomiting Do NOT induce vomiting Give plenty of water Get medical attention Other (specify):

DERMAL Flush with soap and water Get medical attention Contaminated clothing - remove & launder Contaminated shoes - destroy Other (specify):

EYE CONTACT Flush with plenty of water for at least 15 minutes Get medical attention Other (specify):

INHALATION Remove to fresh air If not breathing, give artificial respiration Give oxygen Get medical attention Other (specify):

VENTILATION REQUIREMENTS - Always maintain exposure below permissible exposure limits
 Consult an industrial hygienist or environmental health specialist Local exhaust Use with adequate ventilation Check for air contaminant and oxygen deficiency

OTHER (specify):

EYE Face shield Goggles Safety glasses
HAND (GLOVE TYPE) Polyvinyl chloride Neoprene Butyl rubber Polyvinyl alcohol Polyethylene Other (specify):

RESPIRATOR TYPE - Use only NIOSH approved equipment:
 Self-contained Supplied air Can or cartridge gas or vapor Filter - dust, fume, mist Other (specify):

OTHER PROTECTIVE EQUIPMENT
 Rubber boots Apron Other (specify):

PRECAUTIONARY LABELING
 Wash thoroughly after handling Do not get in eyes, on skin or clothing Do not breathe vapor Keep container closed Keep away from heat, sparks, and open flames Store in tightly closed containers

Do not store near combustibles Keep from contact with clothing and other combustible materials Empty container may contain hazardous residues Use explosion proof equipment Other (specify):

Other handling and storage instructions:

Prepared by: Christie B. Johnson Date: 10/15/82 Address: Three Parkway, Phila., PA 19102 Phone: 215/587-7550

PLEASE NOTE: The above information is accurate to the best of our knowledge. However, since data, safety standards, and government regulations are subject to change and the conditions of handling and use of this material are beyond our control, Pennwalt MAKES NO WARRANTY, EITHER EXPRESS OR IMPLIED, WITH RESPECT TO THE COMPLETENESS OR CONTINUING ACCURACY OF THE INFORMATION CONTAINED HEREIN AND DISCLAIMS ALL LIABILITY FOR RELIANCE THEREON. User should satisfy himself that he has all current data relevant to his particular use.

HEALTH HAZARD INFORMATION

SPECIAL PROTECTION INFORMATION

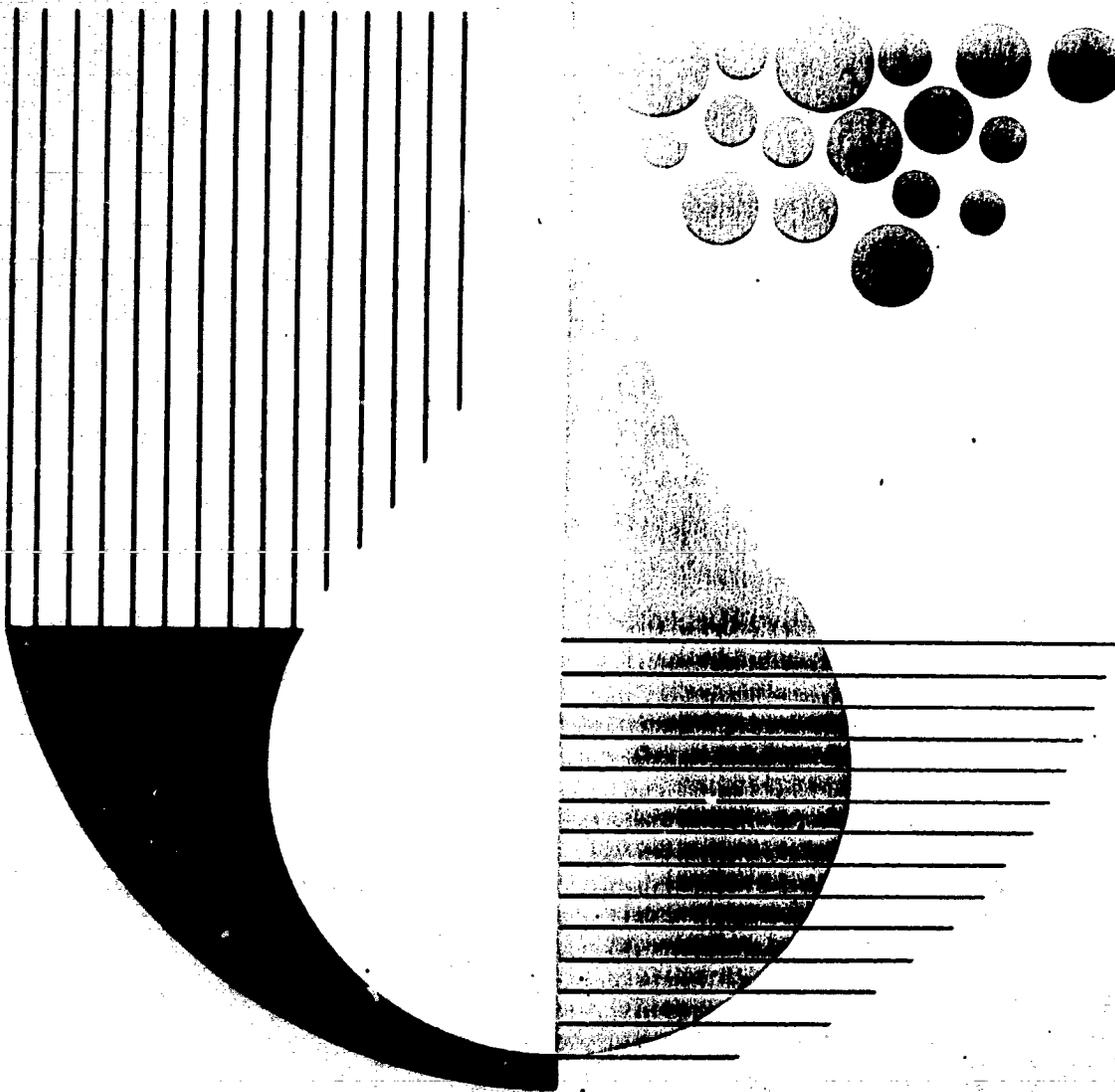
SPECIAL PRECAUTIONS

0014

PENWALT

PENNAD 150

boiler water additive
for corrosion control
in condensate lines



0015

Introduction

Authorities in the field of boiler water treatment have long recognized the necessity for controlling corrosion in steam condensate lines.

Such corrosion is normally caused by low condensate pH due to dissolved carbon dioxide. It can therefore be effectively reduced by the use of a volatile neutralizing amine which functions to keep condensate pH slightly on the alkaline side. PENNAD® 150 (diethylamine/ethanol) has been proven to be effective in this application.

Physical and chemical properties of PENNAD 150, general information on use in steam condensate systems, and results of comparison tests with other volatile amines are given in this bulletin. Additional information is available upon request.

FDA Allowance

Diethylaminoethanol has been included in the Food Additive Regulations Section 121.1088 for use in steam which comes in contact with food products, excluding milk and milk products. The FDA allowance for concentrations up to 15 ppm was obtained by rigorously controlled feeding studies. This concentration is higher than the maximum 10 ppm safely allowed for morpholine and cyclohexylamine under their "Generally Recognized As Safe" (GRAS) rating.

Cost-Performance

Recent tests in actual commercial steam generating systems have shown that PENNAD 150 has cost-performance characteristics superior to other volatile amines, such as morpholine and cyclohexylamine, commonly used for this purpose.

It is generally recognized that neither morpholine nor cyclohexylamine provides the optimum in economical protection. For this reason, industry has recommended and supplied various blends of these two amines for this application. PENNAD 150, however, combines in a single product many of the advantages of the blend — yet eliminates many of the problems and uncertainties involved in adding two amines which will be lost from the system at different rates.

Because it exhibits good stability at 1500 psi and steam temperatures up to 800°F, PENNAD 150 may also be considered for use in power plant steam generating systems.

Some of the properties of PENNAD 150 which are most important in its performance as a neutralizing amine are shown in the table opposite.

Physical and Chemical Properties of Volatile Neutralizing Amines for Steam Condensate Systems

	PENIAD® 180 Diethylamine/ethanol	Morpholine	Cyclohexylamine
Boiling Point*	325°F	264°F	275°F
Azeotropic Point at 760 mm Hg		None	
Boiling Point	210°F		205°F
% Amine in Vapor	25		
Open Cup Flash Point*	135°F	102°F	90°F
Basicity			
K_b	52×10^{-4}	2.4×10^{-3}	1.5×10^{-3}
Approx. pH of 0.001 N Soln.	10.3	9.8	10.0
Vapor/Liquid Distribution Ratio	1.7	0.4	0.7
Freezing Point*	-70°F	23°F	10°F

*Concentrated (100%) amine

General Information on PENNAD 150 in Steam Condensate Systems

PENNAD 150 is in the class of volatile neutralizing amines. It is stable, and does not break down to form solid products which can restrict flow.

It is generally recognized that each of the major amines now in use is subject to performance defects under certain conditions. Morpholine does not carry to the far ends of a long system, and excessive quantities of it are required for a high pH. It is also subject to excessive blow-down losses compared to the more volatile amines.

Cyclohexylamine, on the other hand, is subject to large deaeration losses, and has been known to cause plugs of solid bicarbonate at the far end of some steam lines.

PENNAD 150, however, has none of these limitations. General information on addition and control are given below.

Dilution

PENNAD 150 is miscible with water in all proportions, and may be added to boiler water in concentrated form, or diluted with water for greater convenience and safety in handling.

The addition of any alkali or amine to hard water containing calcium bicarbonate will form the less soluble calcium carbonate, which will precipitate. This precipitate will normally cause no trouble, but could conceivably clog small lines or strainers. Diluting the amine with softened or deionized water will avoid the formation of the precipitate.

Addition Rate

The amount of PENNAD 150 required for a given system will depend on many factors. These include the amount and composition of the make-up water, whether or not the system includes a deaerator, and the operation of the deaerator if present. Amount of blow-down, amount of condensate recycled, maintenance of adequate alkalinity in

the boiler, and amount of steam generated also affect amine demand.

The "Boiler Water Treatment Manual for Federal Plant Operators" (Handbook 5, pages 58-60) discusses addition of neutralizing amine. Although only cyclohexylamine is mentioned in this discussion, much of it is equally applicable to PENNAD 150. As indicated in the section entitled "Estimating the Dosage for Cyclohexylamine," the amount of CO₂ present in the boiler water, including that present as carbonate and bicarbonate, is a major factor in determining amine demand.

Major changes in the composition or amount of make-up water will also result in marked variations in the amount of amine required.

Sufficient alkalinity of the boiler water must be maintained by addition of a strong base, such as caustic soda. Otherwise, an excessive amount of amine will be trapped in the boiler in the form of phosphates and other stable salts.

Method of Application

PENNAD 150 may be introduced into the steam system in the same way as other condensate corrosion inhibitors. For example, it may be added to a mixture of other boiler water treatment chemicals, such as caustic soda, phosphates, etc. It should always be added downstream from the deaerator to prevent excessive amine loss; if no deaerator is in the system, it may be added at any convenient point.

PENNAD 150 is compatible with other boiler water treatment chemicals in the concentrations in which they are normally fed to the boiler. However, the compatibility of PENNAD 150 should be checked before adding it to any concentrated formulation.

Control

PENNAD 150 reduces corrosion of condensate return lines by neutralizing carbonic acid formed in the condensate due to absorption of CO₂ present in the steam.

The pH of the condensate should not be allowed to drop below 7.0 at any point in the system if adequate protection is to be obtained. Therefore, it is desirable to select a sampling point or points at which the pH is the lowest, and add sufficient PENNAD 150 to the system to maintain the pH above 7.0 at these points. A higher pH of 8.0 or 8.5, of course, gives greater assurance of protection, but also increases cost.

The CO₂ in the steam will tend to concentrate toward the ends of long, low pressure steam lines, and will be absorbed to the greatest extent where the condensate cools in an atmosphere rich in CO₂. Therefore, such locations will ordinarily be the points at which, in the absence of PENNAD 150, the lowest pH will be experienced.

Several methods of pH determination are available. Of course, the pH meter is the most accurate, but also the most expensive.

The Taylor pH Slide Comparator** is a moderately priced instrument which is practical for use in the boiler room.

A. A. Berk and G. L. Hopps in "Return Line Corrosion in Federal Heating Systems" (RI 5929, page 30) describe the preparation and use of a mixed color indicator adapted for pH control of neutralizing amines in steam condensates.

It is desirable to cool condensate samples, particularly if the samples are at or near their boiling point. This cooling should be done in such a way that gaseous portions of the sample are not allowed to escape until after the sample has been cooled. The pH should be determined immediately after collection of the sample if possible.

*Published by the U.S. Dept. of the Interior—Bureau of Mines. Available from the Publications Section, U.S. Bureau of Mines, 4800 Forbes Ave., Pittsburgh, Pa. 15213.

**Manufactured by W. A. Taylor, 7300 York Road, Baltimore, Maryland.

0019

Pennwalt PENNAD® 150* vs. Other Volatile Amines in a 200 psi Deaerated Steam System

	Averages of Daily Additions and Observations		
	PENNAD® 150*	Morpholine	Cyclohexylamine
Amine Added (lbs.)	1.33	1.61	2.26
Amine Concentration (ppm amine based on make-up water ¹)	33	41	62
Steam Production (lbs.)	258,000	280,000	316,000
Make-up Water Added ¹ (% of steam produced)	15.5	12.1	11.4
CO ₂ ² in Make-up Water ¹ (ppm)	30	33	39
Neutralizing Dose Requirement	1.09	1.22	1.57
Condensate Analysis			
pH	7.8	8.0	8.6
CO ₂ ² (ppm)	11.4	11.9	15.4
Alkalinity (as ppm amine)	36	39	45.6
NDHA Test ³ (mils/year)	1.2	0.8	0.6

*PENNAD® 150-Diethylaminoethanol

¹Make-up water from zeolite softener

²CO₂ includes combined CO₂ present in carbonates and bicarbonates

³Wt of Amine Added/Wt of CO₂ in Make-up water

³Less than 10 mils/yr is considered "Negligible Corrosion" in this test

The data at left were taken from a 200 psi de-aerated steam system. Comparison of PENNAD 150 with morpholine in a smaller 8-12 psi boiler (125 H.P.) showed an even greater advantage over morpholine in a non-de-aerated system.

As can be seen from an examination of the table at left and other data presented in this bulletin, PENNAD 150 demonstrates several important advantages over both morpholine and cyclohexylamine.

Advantages of PENNAD™ 150 over Morpholine

- Better protection on longer runs of low pressure steam lines.
- Favors vapor over liquid, giving better protection where CO₂ may accumulate, as at the end of a steam line.
- Is a stronger base than morpholine.
- Results in lower blow-down losses.
- Has higher flash point than morpholine, permitting safer handling.
- FDA allows 50% higher concentration of PENNAD 150 than morpholine in steam contacting food products.

Advantages of PENNAD™ 150 over Cyclohexylamine

- No tendency for PENNAD 150 to form a solid reaction product with CO₂ as occurs with cyclohexylamine under certain conditions, avoiding possible clogging of small orifices and strainers.

- Lower de-aerator loss from de-aerated systems.
- Better protection in high temperature condensate.
- Has higher flash point than cyclohexylamine, permitting safer handling.
- FDA allows 50% higher concentration of PENNAD 150 than cyclohexylamine in steam contacting food products.

Handling and Storage of PENNAD™ 150

Concentrated PENNAD 150 should be handled with the same precautions as other concentrated amines having a flash point over 100°F. Contact with the skin, and particularly the eyes, should be avoided.

Toxicology of PENNAD™ 150

FDA regulations permit up to 15 parts per million of PENNAD 150 (diethylaminoethanol) in steam which contacts food, with the usual exception of milk and milk products. This 15 ppm limit for PENNAD 150 is 1½ times the maximum permitted for either morpholine or cyclohexylamine. Since each formulation under its specific trade designation must be approved for use in meat processing and in poultry processing plants, approval for these applications is the responsibility of the formulators.

NOTICE

The information contained herein is, to the best of our knowledge and belief, accurate. Since the conditions of handling are beyond our control, we make no guarantee of results. We assume no liability for damage or liability resulting from following our suggestions or recommendations, nor are there any implied warranties or recommendations to infringe any patent.

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PENNWALT CORPORATION • ORGANIC CHEMICALS DEPARTMENT • PHILADELPHIA, PENNSYLVANIA 19102



LABORATORY REPORT

CONFIDENTIAL: PENNSALT CHEMICAL CORPORATION

RE: SENSITIZATION STUDIES WITH DIMETHYLAMINO-ETHANOL (DMAE)
AND WITH DIETHYLAMINO-ETHANOL (DEAE)

THE SKIN SENSITIZATION POTENTIALS OF DMAE AND OF DEAE HAVE BEEN DETERMINED USING THE GUINEA PIG AS THE EXPERIMENTAL ANIMAL. BOTH PRODUCTS WERE STRAW-COLORED LIQUIDS AND WERE RECEIVED BY THIS LABORATORY 12/16/57; THEY WERE REGISTERED BY US AS PR 571282 AND PR 571283, RESPECTIVELY.

METHOD.

THE EXPERIMENTAL METHOD WAS THAT DESCRIBED BY DIAIZE, HOODARD AND CALVERY (J. PHARMAC. & EXPER. THER. 82, 377-390, 1944). EACH COMPOUND WAS DISSOLVED IN DISTILLED WATER AT A CONCENTRATION OF 0.1% AND INJECTED INTRADERMALLY IN TEN GUINEA PIGS; INJECTIONS WERE REPEATED EVERY OTHER DAY UNTIL A TOTAL OF TEN WERE ADMINISTERED. TWO WEEKS AFTER THE LAST INJECTION, EACH ANIMAL WAS GIVEN A "CHALLENGE" INJECTION AND EXAMINED TWENTY-FOUR HOURS LATER TO RECORD THE DIAMETER, HEIGHT AND COLOR REACTION; THESE RATINGS WERE THEN COMPARED WITH SIMILAR RATINGS WHICH WERE RECORDED FOLLOWING THE FIRST INJECTION.

RESULTS.

OBSERVATIONAL DATA ARE PRESENTED IN THE ACCOMPANYING LABORATORY REPORT FORMS. WITH EACH OF THE TWO COMPOUNDS, THE RESPONSE TO THE CHALLENGE INJECTION WAS LESS THAN THE RESPONSE TO THE INITIAL INJECTION. IT IS CONCLUDED THEREFORE THAT NEITHER DMAE NOR DEAE IS A SENSITIZING AGENT; THE FINDINGS DO NOT SUGGEST THAT EITHER COMPOUND POSSESSES ANY SIGNIFICANT CONTACT DERMATITIS POTENTIAL.

PHARMACOLOGY RESEARCH, INC.
MARCH 13, 1958.

M. J. ...
Maria ...

PHARMACOLOGY RESEARCH, INC.
DARBY, PA.

LABORATORY REPORT

CODE: PR # 57-1282 LABEL ^{IN 2928} DIMETHYLAMINO - ETHANOL PF 281 CODE S 513
DATE REC'D 12/16/57 SOURCE PENNSALT CHEMICAL CORPORATION

TEST: **SENSITIZATION STUDY - GUINEA PIGS.**

METHOD: **DRAIZE, WOODARD & CALVERY**

RESULTS.

GUINEA Pigs No.	INITIAL SCORE			FINAL (CHALLENGE) SCORE		
	DIA. MM	HT. MM	COLOR	DIA. MM	HT. MM	COLOR
11	5	0	2	3	0	1
12	7	0	1	5	1	1
13	6	0	1	5	0	0
14	6	0	1	6	1	1
15	6	1	2	6	1	0
16	6	0	1	0	0	0
17	6	0	1	4	0	0
18	6	0	2	6	0	0
19	6	0	1	5	0	1
20	6	0	1	0	0	0
Av.	6	0	1	4	0	0

CONCLUSION:

THIS PRODUCT IS A NON-SENSITIZING AGENT.

PHARMACOLOGY RESEARCH, INC.

BY MARIE DUGAN
DATE 3/13/58

PROTOCOL REF. MLD I, 2,3.

0 0 2 4

PHARMACOLOGY RESEARCH, INC.

DARBY, PA.

LABORATORY REPORT.

CODE: PR # 57-1283 ^{MN 2160} LABEL DIETHYLAMINO - ETHANOL FF 282
 DATE REC'D 12/16/57 SOURCE PENNSALT CHEMICAL CORPORATION

TEST: **SENSITIZATION STUDY - GUINEA PIGS.**

METHOD: **DRAIZE, WOODARD & CALVERY**

RESULTS:

GUINEA Pig No.	INITIAL SCORE			FINAL (CHALLENGE) SCORE		
	DIA. MM	HT. MM	COLOR	DIA. MM	HT. MM	COLOR
1	6	0	0	5	0	0
2	5	0	1	3	0	1
3	6	0	1	0	0	0
4	4	0	1	3	0	1
5	6	0	1	2	0	0
6	8	1	1	4	0	0
7	6	0	1	5	1	1
8	7	1	1	5	0	1
9	6	1	1	0	0	0
10	6	0	1	2	0	0
Av.	6	0	1	3	0	0

CONCLUSION:

THIS PRODUCT IS A NON-SENSITIZING AGENT.

PHARMACOLOGY RESEARCH, INC.

BY M. DUGAN

DATE 3/13/58

PROTOCOL REF. MD: I, 2, 3.

0025

TOXICOLOGY REPORT
FOR PENNWALT CORPORATION

RE: DIETHYLAMINOETHANOL #0129.

A CLEAR, COLORLESS LIQUID.

SUMMARY. (1) EYE IRRITANCY IN RABBITS: CORROSIVE (UNWASHED AND WASHED).
(2) DOT SKIN CORROSIVITY IN RABBITS: NONCORROSIVE.

(1) EYE IRRITANCY IN RABBITS.

METHOD. ONE-TENTH ML OF SAMPLE WAS PLACED IN THE CONJUNCTIVAL SAC OF ONE EYE OF EACH OF SIX ALBINO RABBITS. WITH THREE OF THESE ANIMALS, THE TREATED EYE WAS WASHED WITH FLOWING WATER INITIATED 20 TO 30 SECONDS AFTER INSTILLATION AND CONTINUED FOR ONE MINUTE. THE IRRITANT REACTIONS WERE SCORED FOR SEVEN DAYS.

RESULTS. THE REACTION INCLUDED ALL OCULAR TISSUES. INSTILLATIONS EVOKED INTENSE PAIN.

UNWASHED. THE CORNEA OPACIFIED PROMPTLY AND COMPLETELY OBSCURED THE PUPIL AND IRIS. THE CONJUNCTIVAE BECAME COMPLETELY NECROTIC (BLACK) WITH MINIMAL SWELLING. IN ADDITION, PATCHES OF NECROSIS APPEARED ON THE EYELIDS. NO SIGNS OF RECOVERY WERE EVIDENT SEVEN DAYS LATER.

WASHED. CORNEAL OPACIFICATION DEVELOPED MORE SLOWLY. DURING THE FIRST TWO HOURS, THE PUPIL WAS CONSTRICTED AND THE IRIS WAS SEVERELY CONGESTED; AT THREE AND FOUR HOURS, THE IRIS REACTED SLUGGISHLY TO LIGHT AND SUBSEQUENTLY FAILED TO REACT AT ALL. INITIALLY THE CONJUNCTIVAE WERE SEVERELY INFLAMED WITH MINIMAL SWELLING AND WITH PATCHES OF NECROSIS PRESENT; THEY WERE COMPLETELY NECROTIC (WHITE) WITHIN 24 HOURS. A WHITE DISCHARGE APPEARED AT THIS TIME. NO SIGNS OF RECOVERY WERE EVIDENT.

COMPARATIVE SCORES WERE AS FOLLOWS (C = CORNEA, I = IRIS, R = CONJUNCTIVAL REDNESS, CH = CHEMOSIS):

TIME	UNWASHED				WASHED			
	C	I	R	CH	C	I	R	CH
1 HR	4	?	3 ^N	1	2	1*	3 ^N	1
2 HRS	4	?	N	1	2	1*	3 ^N	1
3 HRS	4	?	N	1	2	1**	3 ^N	1
4 HRS	4	?	N	1	2	1**	3 ^N	1
24 HRS	4	?	N	1 E	2	2†	N	1 D
48 HRS	4	?	N	1 E	>2	2†	N	1 D
72 HRS	4	?	N	1 E	>2	2†	N	1 D
4 DA	4	?	N	1 E	3	?	N	1 D
5-7 DA	4	?	N	1 E	3	?	N	1 D

(CONTINUED)

EYE CODE: * MIOSIS.
** SLUGGISH LIGHT REACTION.
† MYDRIASIS, NO LIGHT REACTION.
N PATCHES OF NECROSIS.
N COMPLETE NECROSIS.
D DISCHARGE.
E PATCHES OF NECROSIS ON EYELIDS.

(2) DOT SKIN CORROSIVITY IN RABBITS.

METHOD. AS PRESCRIBED IN 49 CFR 173.240 (SIX ALBINO RABBITS, FOUR HOUR SKIN-CONTACT TIME, 48 HOURS OBSERVATION).

RESULTS. WHEN EXPOSURES WERE TERMINATED, ALL TREATED SITES WERE DARK GRAY IN COLOR WITH A RED SURROUND AND WITH SLOUGHED PATCHES OF SURFACE EPITHELIUM. SUBSEQUENTLY THE SITES BECAME THICK (HYPERTROPHY) AND DRY BUT REMAINED SUPPLE. NO SIGNS OF DERMAL DESTRUCTION WERE EVIDENT.

PHARMACOLOGY RESEARCH, INC.

By A. R. Latven
A. R. LATVEN 8/01/77

PROTOCOL REFS: PR#77-5367; (1) RS I, 37; (2) DO, 31.

PENNSALT CHEMICALS CORPORATION
Product Applications Laboratory
900 First Avenue
King of Prussia, Pennsylvania 19406
Rec'd 1/9/67

FINAL REPORT

ON

One-Year Chronic Feeding in Beagle Dogs

of

Diethylaminoethanol

FOR

**Pennsalt Chemicals Corporation
King of Prussia, Pennsylvania**

By: *John Eibert, Jr.*
John Eibert, Jr., Ph.D.
President and Director
Biological Research Division

Collaborators:

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Date: December 30, 1966

S.A. Number 101333

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0 0 2 9

I. SYNOPSIS:

- A. Two groups of Beagle dogs (consisting of three males and three females each) were fed Diethylaminoethanol for 365 days at dietary levels of 500 ppm* (Test Low Level) and 1,000 ppm (Test Intermediate Level), respectively. Another group of animals of similar size was fed DEAE 5,000 ppm (Test High Level) in the diet for days 1 through 39 of the study and at 2,000 ppm via gelatin capsules to survivors for the 134th day through termination of the study. A fourth group of six animals was fed at a dosage level of 10,000 ppm DEAE until death occurred in all animals. A control group of dogs (consisting of three males and three females) was fed the basal laboratory dog meal without the test compound.
- B. None of the test animals of Group I (500 ppm) displayed gross signs of ill effects during the entire study. All animals of Group II (1,000 ppm) exhibited at various times tremors and/or shaking of the head from side to side. These signs which were of slight intensity and which intermittently occurred were manifested more strongly in dog numbers 8 and 9 throughout the study. All dogs of Group III (5,000 ppm) and Group IV (10,000 ppm) exhibited severe cases of weakness, tremors, convulsions and ataxia with two animals at the 5,000 ppm test level succumbing (day 35 and 41 respectively) and all animals at the 10,000 ppm test level succumbing between days 18 and 35 of the study.
- C. During the period between days 39 and 134 when the animals of Group III (5,000 ppm) were returned to normal diet, the four survivors showed gradual improvement, however; severe ataxia and intermittent tremors were still evident upon resumption of administration of the test material by capsule on the 134th day of the test. All animals displayed a slight increase in ill effects immediately following resumption of the dosage at 2,000 ppm but gradually developed a tolerance for the test compound and showed slight improvement, however, severe ataxia and tremors persisted in all throughout the study.
- D. Body weight and food consumption records of all animals of Group I (500 ppm) and Group II (1,000 ppm) appeared normal and comparable to the control animals during the study.
- E. With the exception of occasional aberrant values in both control and test groups, no significant hematological changes were evident in the test animals as compared to the controls and the findings were considered to be within normal limits.
- F. Urine analyses showed occasional aberrant values but no significant differences between the test and control groups were noted.

* DEAE as the free base

- G. Plasma biochemistry analyses showed occasional aberrant values but no significant differences between the test and control groups were noted.
- H. With the exception of the findings noted in moribund animals of Group III (5,000 ppm) and Group IV (10,000 ppm) clinical examinations showed no abnormalities with respect to pulse rate, reflexes, condition of mucous membranes and auscultation which could be related to dietary feeding of the test preparation. Evaluation of electrocardiographic tracings indicated no detectable damage to the conduction system of the heart which could be attributed to or connected with administration of DEAE.
- I. Gross necropsy of the animals which succumbed during the first 180 days of the study showed congestion and diffuse hemorrhages of the lungs, congestion of the kidneys, reddish mottled coloration of the spleen, hardness of the liver and numerous enlarged and congested lymph nodes. One or more of these lesions were observed in the majority of the animals. Gross necropsy of the surviving animals sacrificed at termination revealed no gross pathological changes which could be attributed to the inclusion of the test compound in the diets or administration of the compound by capsule.
- J. Occasional aberrant organ weights were obtained in animals of each group, including the controls, however, the overall organ weight values for the test and control dogs were comparable.
- G. Microscopic examination of tissue sections showed atrophy of the thyroid glands and gonads of dogs of Group III (Test High Level) which were interpreted as a non-specific secondary response to the metabolic or toxic insult of the test compound at this dosage level. Cerebellar changes which were observed in this group were considered a specific toxic effect associated with the clinically observed tremors and ataxia. No morphologic abnormality was observed in sections of cerebellum from dogs in the low and intermediate test levels. Findings of micropathological examination of tissues from control dogs were within normal limits.

II. INTRODUCTION:

The purpose of this study was to evaluate and characterize the oral toxicity of diethylaminoethanol when fed to dogs for a period of 1 year.

The study was initiated on October 11, 1965 and terminated on October 10, 1966.

A progress report on this study was submitted to the Pennsalt Chemicals Corporation, King of Prussia, Pennsylvania on May 23, 1966.

This final report includes and supplements the data presented in the progress report and provides an overall evaluation of the results obtained.

III. MATERIAL:

The sample of test compound used for this study was received from the Pennsalt Chemicals Corporation, King of Prussia, Pennsylvania on October 11, 1965. (Six 1 gallon glass bottles).

The analysis of the compound, according to the inscription and as used in this study, was as follows.

CONCENTRATION - 53.5% DEAE* by weight
70.2% DEAE* HCl by weight

1.000 ml. contains 0.577 gm. DEAE or 0.758 gms. DEAE. HCl

*Diethylaminoethanol

The aqueous solution of DEAE. HCl was a light brown liquid, slightly more viscous than water, with a sweet pungent odor.

IV. METHODS:

A. General Procedure:

Thirty purebred beagle dogs, 15 females and 15 males, which were in apparent good health, were selected for use on this study. The dogs were quarantined for five weeks prior to the beginning of compound administration during which time they were dewormed and immunized against distemper, infectious hepatitis and leptospirosis, and acclimated to laboratory conditions and diet. During the quarantine period, pretest clinical observations and tests were performed, these included records of body weight and general feed consumption, physical examinations (body temperature, reflexes, pulse rate and auscultation) and blood and urine analyses.

The animals were divided into five groups as follows: one control group and four test groups, each group consisting of three females and three males. The dogs were distributed among the groups by litter, weight, sex and age as presented on page 5. Littermates were distributed among the groups whenever possible.

All animals were maintained in a uniform environment and housed in individual cages with access to outdoor runs. All surviving animals were observed daily (five days per week) for toxic and/or pharmacological effects through 365 days. These observations were made both in the cages and in the runs. Body weights were recorded weekly and feed consumption daily (five days per week) for each dog. Diethylaminoethanol was administered daily by mixture with the basal laboratory diet which consisted of ground Purina Dog Meal*. The compound administration was according to the established test concentrations presented on page 5. Diets were freshly prepared each week. Wayne Self-Feeders were used as the feed containers and the respective diets were provided ad libitum. Water was freely available at all times.

* - see following page

* Because of their poor condition and very poor food consumption, all surviving dogs at both the 5,000 ppm and 10,000 ppm test levels were returned on the 39th day of the study to the regular control diet in order to see if the obvious ill effects were reversible. On the 134th day of the study, the four survivors at the 5,000 ppm test level were again challenged with administration of DEAE at a reduced dosage level (2,000 ppm) which was dosed to the animal via gelatin capsules. To determine the proper dosage for these animals, the DEAE concentration was adjusted weekly based on a projection of each of the animals' weight and average daily feed consumption obtained during the previous week.

SCHEMATIC OUTLINE OF STUDY

Group Number	Dietary Level (ppm*)	Animal Number	Sex	Litter	Age at Initiation (Months)	Body Weight at Initiation (kg.)
I	500	1	M	B	4½	5.45
		2	M	A	4½	6.13
		3	M	E	4½	6.92
		4	F	A	4½	4.99
		5	F	P	4½	6.02
		6	F	N	5	6.70

II	1,000	7	M	D	4½	5.90
		8	M	O	4½	6.02
		9	M	M	4½	7.15
		10	F	B	4½	4.77
		11	F	P	4½	6.24
		12	F	D	4½	6.02

III	5,000 (Days 1 through 39)	13	M	D	4½	7.83
		14	M	B	4½	6.36
		15	M	D	4½	8.17
	2,000 (Days 134 through termination, via capsule)	16	F	I	5	5.90
		17	F	D	4½	6.24
		18	F	C	4½	5.68

IV	10,000	19	M	L	4½	6.36
		20	M	K	4½	6.92
		21	M	D	4½	8.97
		22	F	J	4½	6.02
		23	F	K	4½	7.49
		24	F	E	4½	6.24

V	0	25	M	M	4½	5.45
		26	M	C	4½	5.22
		27	M	A	4½	6.36
		28	F	G	5	5.22
		29	F	H	5	5.68
		30	F	P	4½	4.65

* All dietary concentrations for this study are calculated on DEAE as the free base

B. Laboratory Tests

1. Hematological Studies:

Blood samples for hematological studies were obtained from each dog prior to purchasing the animals and again during the pre-treatment quarantine period. During the experimental period, samples were taken from each animal at 30, 45, 90, 180 and 360 days. The following studies were performed at each examination interval on each dog: total and differential leukocyte counts, hemoglobin concentration, hematocrit, erythrocyte sedimentation rate and prothrombin time. An exception to this was for the first control analyses, in which the latter two determinations were not performed.

2. Plasma Biochemistry Studies:

Routine determinations on plasma which included quantitative tests for glucose, total protein, total albumin (albumin-to-globulin ratios were calculated) and urea nitrogen were performed on each dog at the second pre-treatment period and at 30, 45, 90, 100 and 360 days. For the first pre-treatment analyses, the quantitative tests for protein were not performed.

3. Liver Function Studies:

Liver function tests which included bromsulphalein retention (BSP), alkaline phosphatase activity, and serum glutamic-oxalacetic transaminase (SGOT) were performed on each dog during the second pre-treatment quarantine period and at 30, 45, 90, 100 and 360 days. SGOT values only, were obtained on each dog for the first pre-treatment period.

4. Urine Analyses:

Urine analyses were performed on each animal during the pre-treatment quarantine period and at 30, 45, 90, 180 and 360 days. Each analyses included albumin, sugar, bilirubin, pH, specific gravity and volume (ml.) determinations and microscopic examination of the sediment. Quantitative determinations were made for total nitrogen.

C. Clinical Observations

A complete physical examination, which included body temperature, pulse rate, reflexes, auscultation and electrocardiograms were performed on each dog, excluding animals from Group IV, (10,000 ppm), at 30, 45, 90, 100 and 360 days.

D. Pathological Studies

1. Necropsy Examination:

Each of the dogs which succumbed during the study was subjected to a complete necropsy which included examination of the organs of the abdominal, thoracic and cranial cavities.

Each of the 22 surviving dogs was sacrificed at 12 months by an intravenous injection of Myotal followed by exsanguination, and a complete necropsy was performed. The following organs from each dog were weighed, and organ/terminal body weight ratios calculated: brain, thyroid, heart, liver, spleen, kidney, adrenal and gonads (males, only).

2. Microscopic Examination:

The following tissues were taken from each animal and preserved in 10 per cent neutral formalin for possible microscopic examination:

brain (3 levels)	pancreas
pituitary	small intestine (3 levels)
spinal cord (3 levels)	large intestine
thyroid	lymph node (cervical & mesenteric)
parathyroid	urinary bladder
lung	testis with epididymis
heart	prostate
liver	ovary
gall bladder	uterus
spleen	bone
kidney	bone marrow
adrenal	striated muscle
aorta	femoral nerve
stomach (2 sections)	any unusual lesion
submaxillary salivary gland	

An exception to this was for Group IV (10,000 ppm) where only organs which showed gross changes at necropsy were preserved in 10% formalin for possible future reference.

The tissues listed above for each control (Group V) and Test High Level (Group III) dog were fixed, paraffin embedded, stained with hematoxylin-eosin, and examined microscopically. In addition, two sections of the cerebellum from each dog of the Test Intermediate (Group II) and Test Low Level (Group I) were prepared and examined microscopically.

V. RESULTS:

A. Appearance, Behavior, Body Weight and Feed Consumption:

Gross signs of toxicity were observed in all of the animals of Group III, (5,000 ppm) and Group IV, (10,000 ppm). The onset occurred in all animals between the 8th and 15th day of the study. The signs included weakness, tremors, twitching, ataxia, violent shaking movements of the head and entire body and occasional convulsive seizures during which the animal appeared to undergo temporary shock. As the study progressed the signs increased in severity with the majority becoming so weakened that they were unable to eat unassisted. Eight of the animals became moribund and succumbed as listed below:

<u>Animal Number and Sex</u>	<u>Number of Days on Test</u>	<u>Group and Dietary Level</u>
14 - Male	35	III - 5,000 ppm
17 - Female	41	III - 5,000 ppm
19 - Male	31	IV - 10,000 ppm
20 - Male	18	IV - 10,000 ppm
21 - Male	39	IV - 10,000 ppm
22 - Female	32	IV - 10,000 ppm
23 - Female	35	IV - 10,000 ppm
24 - Female	25	IV - 10,000 ppm

Because of the apparent signs of ill effects noted at these levels, it was decided to return the survivors to normal laboratory diet on the 39th day of the study to determine if the damage was reversible. The four survivors, Dogs Nos. 13, 15, 16 and 18 showed gradual improvement after being returned to control diet during days 39 through 134 of the study. This consisted of diminishing of tremors and an increase in overall strength and appetite. Although all of the animals were still severely ataxic and animal number 18 was exhibiting generalized weakness, compound administration (2,000 ppm) via gelatin capsules was resumed to these dogs on the 134th day of the study. The dosage was administered six days per week following feeding of the animals. Following resumption of compound administration by capsules, all animals showed a slight increase in signs of adverse effects, however, after 180 days of the study the dogs slowly developed an apparent tolerance to the compound at this level and a gradual improvement was noted in each. This consisted of an increase in body strength and appetite and a slight decrease in ataxia and tremors, however, pronounced ataxia and occasional tremors persisted in each of the four animals through termination of the study. Dog No. 18, which was unable to stand at 180 days, regained the ability to maintain a standing posture during the second six months of the study.

- 9 -

All animals of Group II (1,000 ppm) exhibited slight tremors and/or occasional shaking of the head from side to side at various times from the 31st to 40th day of the test. The signs subsided in four of the animals by the 130th day of the test, however, Dogs Nos. 8 and 9 continued to show intermittent tremors of slight intensity throughout the study. With the exception of these signs the animals of this group showed normal appetite and otherwise appeared healthy.

The remaining animals of both sexes, in Groups I (500 ppm) and Group V (Controls) ate well and appeared normal and healthy during the entire study. The body weight and feed consumption values for both male and female test animals of Group I and II were generally comparable to the controls. All of the control and test dogs (Groups I and II) showed weight gains and feed consumption within normal limits for this age and breed of dog. The individual weekly body weights and feed consumption records (compound consumption for test groups) are presented in Table 1.

B. Laboratory Tests: - Hematological Studies, Liver Function and Plasma Biochemistry Tests and Urine Analyses

The results of the hematological studies (Table 2), the urine analyses (Table 3) and the liver function and plasma tests (Table 4) indicated no adverse effects due to the dietary feeding (or administration by capsule) of the test compound. The high SGOT values obtained in the majority of dogs on the first control interval are attributed to hemolysis of the blood during shipment from the kennel from which the animals were purchased, since subsequent control SGOT values generally were within normal limits.

Aberrant results were occasionally obtained with each test group and the controls, at each of the examination intervals, however, the values for the control and test dogs were comparable and were considered generally to be within normal limits.

C. Clinical Observations:

Weakened pulse and dried mucous membranes were noted in all moribund dogs of Group III (5,000 ppm) and Group IV (10,000 ppm). With the exception of these findings, the remaining animals at each of the test levels and the control dogs revealed results of physical examinations which were generally within normal limits. Due to the severe ataxia and tremors evident in the four dogs of Group III (5,000 ppm), it was not possible to produce legible electrocardiographic tracings at the 180 day interval. Prior to sacrifice at termination (12 months) satisfactory electrocardiograms were performed on these dogs under anesthesia.

The electrocardiographic records of all surviving dogs at termination showed essentially normal conductive mechanisms in each animal. Dogs Nos. 8, 9 and 10 which showed possible minor heart damage, unrelated to the administration of DEAE, at earlier testing intervals showed normal recordings at the 360 day interval.

Based upon the results obtained from the electrocardiographic tracings of these animals, it is established that DEAE, at the levels fed caused no damage to the conductive mechanism of the heart.

D. Pathological Studies:

1. Necropsy Findings:

The results of gross examination of animals which succumbed and following sacrifice at 12 months are presented in Table 6.

Gross necropsy of the dogs which succumbed showed congestion and diffuse hemorrhages of the lungs, congestion of the kidneys and numerous enlarged and congested lymph nodes. One or more of these lesions were observed in the majority of the animals.

Gross necropsy of the dogs sacrificed at termination showed minimal sporadic lesions in all groups, including the controls, which included mesenteric lymph node enlargement and congestion, urinary bladder inflammation and thickening, and small hemorrhagic lesions of the ileocolic sphincter. These findings could not be correlated by dietary level and were considered to be incidental and unrelated to the feeding of the test compound.

2. Organ Weights:

Terminal body weights, organ weights and organ/terminal body weight ratios are presented in Table 5. Inspection of the data revealed occasional abnormal values in each group including the controls, however, the overall findings for all of the test groups were comparable to the control animals.

3. Microscopic Findings:

The results of the microscopic examination of tissues of the dogs are presented in Table 6.

A summarization of the histopathological evaluation of tissues is as follows:

The tissues of the control group dogs were essentially normal, with one male and one female exhibiting mild lymph node hyperplasia.

The sections of cerebellum from the 12 dogs in the low and intermediate dosage groups were interpreted as normal and exhibited no morphologic differences from those of the six control group animals.

Dogs of Group III (Test High Level) exhibited a number of significant pathologic abnormalities. Thyroid atrophy of mild to moderately severe degree was found in one male and all three females. Testicular atrophy of mild to moderate proportions was found in the three male dogs, and some decrease in oogenesis was present in one of the female animals. Male dog No. 14 which died early in the study also exhibited extensive bronchopneumonia and an associated acute splenic reaction. Two males exhibited acute lymphadenitis. One female showed hydropic change in the renal loops of Henle, and one female exhibited a small cerebral cortical glial nodule.

Conspicuous pathologic abnormalities were present in the sections of cerebellum in the three male dogs and one of the three female dogs in Group III. These changes consisted of irregular patchy degeneration and loss of small to moderate numbers of Purkinje cells, with occasional corresponding mild decrease in cellularity of some areas of the granular cell layer. Foci of tissue calcification were present in the cerebellum of the affected female dog.

Evaluation:

The atrophy noted in the thyroid glands and gonads of the animals of Group III (Test High Level) was interpreted as a non-specific secondary response to the metabolic or toxic insult offered by the experimental feeding program. The cerebellar changes observed in this group were considered a specific toxic effect which represented the morphologic concomitant of the clinically observed tremors and ataxia. No morphologic abnormality was found in the comparable sections of cerebellum from dogs in the low and intermediate test groups.

EFFECTS INFORMATION PROFILE

NOV 19 1983

ID No.	CHEMICAL NAME	SYNONYMS	CAS No.															
90	Ethanol, 2-(diethylamino)-	N,N-diethylethanolamine; 2-hydroxytriethylamine	100-37-8															
Description Colorless, corrosive, hygroscopic liquid; amine-like odor		Use Corrosion inhibitor, emulsifier for polishes; curing agent for resins; fabric softener																
Melting point: -70°C Vapor pressure (B.P.): 21mm HG at 20°C (101°C) Specific gravity: 0.884 (20/20°C) Water solubility: Soluble Organic solubility: Sol. in alcohol, benzene, ether Log P oct/water: -0.73 Empirical formula: C ₆ H ₁₅ NO		Structural Formula $ \begin{array}{c} \text{C}_2\text{H}_5 \\ \diagdown \\ \text{N} - \text{CH}_2\text{CH}_2\text{OH} \\ \diagup \\ \text{C}_2\text{H}_5 \end{array} $																
Biochemical Information <table border="1"> <thead> <tr> <th>Reference</th> <th>Nature of Info.</th> <th>Page</th> </tr> </thead> <tbody> <tr> <td></td> <td></td> <td></td> </tr> </tbody> </table>		Reference	Nature of Info.	Page				Observations in Humans <table border="1"> <thead> <tr> <th>Reference</th> <th>Nature of Info.</th> <th>Page</th> </tr> </thead> <tbody> <tr> <td>Patty (1963)</td> <td>Metabolism</td> <td>4</td> </tr> </tbody> </table>		Reference	Nature of Info.	Page	Patty (1963)	Metabolism	4			
Reference	Nature of Info.	Page																
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Toxicological Information <table border="1"> <thead> <tr> <th>Reference</th> <th>Nature of Info.</th> <th>Page</th> </tr> </thead> <tbody> <tr> <td>CAF</td> <td>LD₅₀; Mutagenicity testing; eye and skin irritation</td> <td>2</td> </tr> <tr> <td>ACGIH (1971)</td> <td>Toxicity review</td> <td>3</td> </tr> </tbody> </table>		Reference	Nature of Info.	Page	CAF	LD ₅₀ ; Mutagenicity testing; eye and skin irritation	2	ACGIH (1971)	Toxicity review	3	Environmental Information <table border="1"> <thead> <tr> <th>Reference</th> <th>Nature of Info.</th> <th>Page</th> </tr> </thead> <tbody> <tr> <td>Verschueren (1977)</td> <td>Effect on fish</td> <td>5</td> </tr> </tbody> </table>		Reference	Nature of Info.	Page	Verschueren (1977)	Effect on fish	5
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Reference	Nature of Info.	Page																
Verschueren (1977)	Effect on fish	5																
Enclosures		Page																

CURRENT AWARENESS FILE

ETHANOL, 2-(DIETHYLAMINO)- ←

000100378
8201
C6-H15-N-O
117.22
Q2N282

DEAE
DIAETHYLAMINOETHANOL (German)
DIETHYLAMINOETHANOL
beta-DIETHYLAMINOETHANOL
N-DIETHYLAMINOETHANOL
2-(DIETHYLAMINO)ETHANOL
2-N-DIETHYLAMINOETHANOL
beta-DIETHYLAMINOETHYL ALCOHOL
DIETHYLETHANOLAMINE
N,N-DIETHYLETHANOLAMINE
N,N-DIETHYL-N-(beta-HYDROXYETHYL)AMINE
2-HYDROXYTRIETHYLAMINE
S

skn-zbt 10 mg/24H
skn-zbt 500 mg open MLD
eye-zbt 5 mg SEV

ozl-rat LD50:1300 mg/kg
ipz-rat LD50:1220 mg/kg
ipx-mus LD50:308 mg/kg
scu-mus LD50:1561 mg/kg
ivn-mus LD50:188 mg/kg
ias-mus LD50:416 mg/kg

JHTAB 26,269.44
UCDS** 6/11/63
UCDS** 6/11/63

JHTAB 26,269.44
TXAPA9 12,486.68
ARZNAD 9,31.59
ARZNAD 4,649.54
ARZNAD 9,31.59
ARZNAD 9,31.59

TLV-TWA 10 ppm (skin)

DTLVS* 4,140.80

OSHA STANDARD-air:TWA 10 ppm (skin) (SCP-J)

FEREAC 39,23540.74

"NIOSH MANUAL OF ANALYTICAL METHODS" VOL 4 270*, VOL 5 S140*

NIMAM*

REPORTED IN EPA TSCA INVENTORY, 1980

RCRVAB 38,975.69
ON-LINE-TOXICOLOGY DATA BANK-NLM, DECEMBER 1982

NIOSH PROFILE (ALKANOLAMINES), SRC, 5/81

NOHS 23774 estimated people exposed, ACT 2%, TRN 98%, GEN 0%, No. OCCS 39

EPA TSCA 8(a) PRELIMINARY ASSESSMENT INFORMATION PROPOSED RULE COMPLETED ← FEREAC 45,13646.80

salmonella microsomal

Used as a corrosion inhibitor, emulsifier for polishes and organic intermediate
Used as a curing agent for resins, an emulsifying agent, and as a fabric softener

2-29-80

TOXICOLOGICAL INFORMATION

DIETHYLAMINO ETHANOL - Skin (diethyl ethanolamine)



10 ppm (Approximately 50 mg/m³)

Diethylamino ethanol was studied by Smyth and Carpenter(1) by the Range-Finding (RF) Test. The single dose, oral R.F. LD₅₀ to rats was 1.3 g/kg; the same order of magnitude as ethylene diamine. The skin penetration, R.F. LD₅₀, was 1.0 ml/kg for guinea pigs, the same order of magnitude as methyl "cellosolve." As a primary irritant it can be compared to morpholine, and its action regarding eye injury can be compared to ammonium hydroxide.

Smyth(2) commented that further study indicated a rat oral LD₅₀ of 2.46 (1.88-3.23) g/kg as a 10% water solution and a rabbit skin penetration LD₅₀ of 1.26 (0.85-1.87) ml/kg undiluted. He regarded the major industrial hazard to be eye injury from the fluid (very severe in rabbit from 0.005 ml undiluted, severe from 15% or more in glycol and not severe from 5% in glycol). He suggested a threshold limit value of 10 ppm.

Because of its irritating properties, probably less than those of n-butylamine, a threshold limit value of 10 ppm is suggested.

References:

1. Smyth, H.F., Jr., Carpenter, C.P.: J. Ind. Hyg. & Tox. 26, 269 (1944).
2. Smyth, H.F., Jr.: Unpublished study from personal communication with TLV Committee member (November, 1964).

ACGIH (1971)

0043

OBSERVATIONS IN HUMANS

Metabolism. The metabolism of the amino alcohols has received little attention. Ethanolamine is naturally formed in mammals from serine and is a normal constituent of mammalian urine.⁶³ Forty per cent of N¹⁵-labeled ethanolamine appears as urea in 24 hours when given to rabbits, suggesting it is deaminised. It is also methylated to choline and converted to serine and glycine. Monomethylaminoethanol and dimethylaminoethanol are intermediates in the conversion to choline. Some 33 per cent of diethylaminoethanol injected into man in 1-g. doses is excreted unchanged. The transformation of the remaining portion is unknown. It could be de-ethylated to ethanolamine and thus enter the normal metabolic pathways.⁶

Patty(1963)

ENVIRONMENTAL INFORMATION

***N*-diethylaminoethanol (diethylaminoethanol; *N*-diethylaminoethylalcohol;
2-hydroxydiethylamine)**

$(C_2H_5)_2NC_2H_4OH$

A. PROPERTIES: colorless liquid; m.w. 117.19; b.p. 163°C; v.p. 1.4 mm at 20°C;
v.d. 4.04; sp.gr. 0.88 at 20/4°C.

B. AIR POLLUTION FACTORS: 1 mg/cu m = 0.21 ppm, 1 ppm = 4.87 mg/cu m

-T.L.V.: USSR: 1 ppm = 5 mg/cu m 1972 (n.s.i.) (240)

USA: 10 ppm = 50 mg/cu m skin 1974 (n.s.i.) (77)

BRD: 10 ppm = 50 mg/cu m skin 1974 (n.s.i.) (241)

-Odor: characteristic: quality: amine
hedonic tone: unpleasant

abs. perc. lim.: 0.011 ppm

50% recogn.: 0.04 ppm

100% recogn.: 0.04 ppm

O.I. 100% recogn.: 33,000 (19)

D. BIOLOGICAL EFFECTS:

→ -Fish: creek chub: critical concs: 80-120 mg/l: 24 hr (226)

Verschueren (1977)

0045

N-Cyclohexyl-2-benzothiazolesulfenamide
(CAS: 95-33-0)



Contains No CBI
RECEIVED
REG. CBI
NOV 11 AM 9:16

General Comments

Much of the referenced literature cited in the "Effects Information Profile" prepared by the Interagency Testing Committee on this material appears to be erroneous. In many cases, i.e. pages 3,4,5,7,11,12,13,14, and 15, the literature is discussing another material and not n-cyclohexyl-2-benzothiazolesulfenamide (CBS).

Product Literature

Attached are copies of a Technical Data Sheet and Material Safety Data Sheet for PENNAC® CBS - Pennwalt's product name for n-cyclohexyl-2-benzothiazolesulfenamide.

Annual Production Data and Trends

Confidential Business Information (CBI).
See enclosed envelope marked "TSCA-CBI".

Production Worker Exposure

Pennwalt has no domestic in-plant exposure for CBS since the material is imported already bagged for domestic sale.

Product Use Exposure

Pennwalt is not familiar with personnel exposure during use of this material in the rubber manufacturing process. This exposure information is probably best determined through representatives of the rubber manufacturing industry. Occasional exposure to this material will occur, however, when bags are accidentally broken in transit or in the warehouses.

CBS is consumed by reaction mechanisms during normal processing in the manufacture of rubber. Therefore, human exposure to this material following the rubber manufacturing process is not anticipated.

Environmental Exposure

CBS is unlikely to have any significant environmental exposure because it is consumed through reaction mechanisms during its use in the rubber manufacturing process.

0 0 4 5

N-Cyclohexyl-2-benzothiazolesulfenamide

(CAS: 95-33-0)

Page 2



The most likely routes of entry to the environment are through spillage or breakage, which are not predictable, and residue in bags. The bag residue, if not consumed during disposal by incineration, would amount to less than 1000 lbs. per 200,000 lbs. of starting material per year, assuming that 4 oz. is left in each bag.

Toxicological Data

Pennwalt does not possess any internally generated toxicity data for CBS. The acute oral LD₅₀, 5.3 gm/kg (rat) and acute dermal 7.94 gm/kg (non-lethal, rabbit) information as shown on the attached MSDS suggest a relatively low order of acute toxicity.

0 0 4 7

MATERIAL SAFETY DATA SHEET

"ESSENTIALLY SIMILAR" TO OSHA FORM 20
FORM 4248 (Rev. 9-90)

ADDRESS: Penwalt Corporation

Three Parkway
Philadelphia, PA 19102

Penwalt Product Name: PENMAC CBS - POWDER	Penwalt Code No. 0634
Chemical Name and Molecular Formula: 2-Benzothiazolesulfenamide, N-cyclohexyl- $C_{13}H_{16}N_2S_2$	
Synonyms:	

Emergency Phone Number(s)
Business: **215-587-5550**
Other: **313-285-9200**

CAS No.(s) **95-33-0**

Chemical Family
Aryl Cyclic Sulfur Amide

MATERIALS OR COMPONENTS	HAZARD DATA (TLV, LD50, LC50, etc.)
N-Cyclohexyl-2-benzothiazolesulfenamide	See Toxicity Section

Description on Shipping Papers - Rubber Accelerators or Softeners, NOIEN
Containers: 50 lbs. net paper bag
175 lbs. net fiber drum

Boiling Point/Range °C °F	Melting Point 94 °C 201 °F	Freezing Point °C °F	Molecular Weight (Calculated) 264.4
Specific Gravity (H ₂ O=1) 1.24-1.30 @ 25 / 25 °C	Vapor Pressure (mm Hg) @ °C °F	Vapor Density (Air=1)	
Solubility in H ₂ O negligible	% Volatiles by Volume 1.0 max.	Evaporation Rate <input type="checkbox"/> Ether = 1 <input type="checkbox"/> Water = 1 <input type="checkbox"/> Butylacetate = 1	
Appearance and Odor Light tan to buff powder		Other	

Flash Point Nonflammable °C °F	Test Method	Flammable Limits Lower % Upper %	Autoignition Temperature/Fire Point °C °F
EXTINGUISHING MEDIA <input type="checkbox"/> Water-spray <input type="checkbox"/> Water-fog <input type="checkbox"/> Water stream <input type="checkbox"/> CO ₂ <input type="checkbox"/> Dry chemical <input type="checkbox"/> Alcohol foam <input type="checkbox"/> Foam <input type="checkbox"/> Earth or sand			

SPECIAL FIRE FIGHTING PROCEDURES
 Do not enter building Allow fire to burn Water may cause frothing Do not use water

UNUSUAL FIRE AND EXPLOSION HAZARDS
 Dust explosion hazard Sensitive to shock Contamination Temperature Other (specify): **SO₂ is a product of combustion.**

STABILITY <input checked="" type="checkbox"/> Stable <input type="checkbox"/> Unstable	CONDITIONS CONTRIBUTING TO INSTABILITY <input type="checkbox"/> Thermal decomposition <input type="checkbox"/> Photo degradation <input type="checkbox"/> Polymerization <input type="checkbox"/> Contamination
---	--

INCOMPATIBILITY - Avoid contact with
 Strong acids Strong alkalis Strong oxidizers Other (specify):

HAZARDOUS DECOMPOSITION PRODUCTS - THERMAL AND OTHER (list)
CO, CO₂, NO_x, SO₂ (if involved in fire)

CONDITIONS TO AVOID
 Heat Open flames Sparks Ignition sources Other (specify):

STEPS TO BE TAKEN IF MATERIAL IS RELEASED OR SPILLED
 Flush with water Absorb with sand or inert material Neutralize Sweep or scoop up and remove Keep upwind. Evacuate enclosed spaces. Prevent spread or spill
 Dispose of immediately Other (specify):

WASTE DISPOSAL METHOD - Consult federal, state, or local authorities for proper disposal procedures.

CONTINUED ON REVERSE SIDE

NA - Not Applicable.

0048

Before using product, read and follow directions and cautions on product label and packaging.

Oral (acute) **LD50: 5.3 gms./kg. (rat)**

Dermal (acute) **7.94 gms./kg. (rabbit) was non-lethal. Not a skin irritant.**

Eye **Slight irritant** Inhalation (acute) **Discomfort from "inert" dust**

Chronic, Subchronic, etc.

PERMISSIBLE EXPOSURE LIMIT (Specify if TLV/TWA or Ceiling (c))
 ACGIH 19 OSHA 19 Other: **Not established**

IRRITATION Skin Severe Moderate
 Eye Severe Moderate Mild (transient)

CORROSIVITY Skin 4 hrs. (DOT) 24 hrs. (CPSC)
 Eye May cause blindness

SENSITIZATION Skin Respiratory Allergen
 INHALATION EFFECTS Narcotic effect Cyanosis Asphyxiant

LUNG EFFECTS (Specify):

OTHER (Specify):
 Repeated contact - skin defatter Other (Specify):

INGESTION Induce vomiting Do NOT induce vomiting Give plenty of water Get medical attention Other (specify):

DERMAL Flush with soap and water Get medical attention Contaminated clothing remove & launder Contaminated shoes - destroy Other (specify):

EYE CONTACT Flush with plenty of water for at least 15 minutes Get medical attention Other (specify):

INHALATION Remove to fresh air If not breathing, give artificial respiration Give oxygen Get medical attention Other (specify):

VENTILATION REQUIREMENTS - Always maintain exposure below permissible exposure limits
 Consult an industrial hygienist or environmental health specialist Local exhaust Use with adequate ventilation Check for air contaminant and oxygen deficiency

Other (specify):

EYE Face shield Goggles
 HAND (GLOVE TYPE) Butyl rubber Polyvinyl alcohol Other (specify):
 Safety glasses Goggles Polyvinyl chloride Neoprene Natural rubber Polyethylene

RESPIRATOR TYPE - Use only NIOSH / MESA approved equipment
 Self-contained Supplied air Can or cartridge gas or vapor Filter - dust Other (specify):

OTHER PROTECTIVE EQUIPMENT
 Rubber boots Apron Other (specify):

PRECAUTIONARY LABELING
 Wash thoroughly after handling Do not get in eyes, on skin or clothing Do not breathe dust Keep container closed Keep away from heat, sparks, and open flames Store in tightly closed containers
 Do not store near combustibles Keep from contact with clothing and other combustible materials Empty container may contain hazardous residues Use explosion proof equipment Other (specify):

Other handling and storage conditions

Prepared by **Christie B. Johnson** Date **11/24/80** Address **3 Parkway, Phila., PA 19102** Phone **215-587-7550**

PLEASE NOTE: "The above information is accurate to the best of our knowledge. However, since data, safety standards, and government regulations are subject to change and the conditions of handling and use, or misuse are beyond our control, Penwalt MAKES NO WARRANTY, EITHER EXPRESS OR IMPLIED, WITH RESPECT TO THE COMPLETENESS OR CONTINUING ACCURACY OF THE INFORMATION CONTAINED HEREIN AND DISCLAIMS ALL LIABILITY FOR RELIANCE THEREON. User should satisfy himself that he has all current data relevant to his particular use."

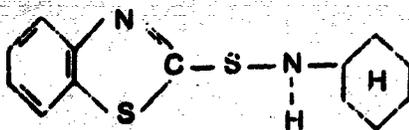
0049

RUBBER ACCELERATORS

PENNAC CBS-0

00739

FORMULA



CHEMICAL NAME

N-cyclohexyl-2-benzothiazole-sulfenamide
(CAS.: 95-33-0)

PROPERTIES

Molecular Weight 264.4
Specific Gravity 1.27
Oil treated to reduce dust in handling

SPECIFICATIONS

Appearance off-white powder
Melting point 95°C min.
Oil content 1.5 ± 0.5%
Ash 0.5% max.
Moisture 0.5% max.
Free amine 1.0% max.
Insoluble in methanol 2.0% max.
Fineness (thru 30 mesh) 99.5% min.

APPLICATIONS

Delayed action accelerator for NR, SBR. Non staining.

PACKAGING

25 kg. (55 lbs.) net weight
Paper bags with PE laminated inner liner
Palletized on wooden pallets.

SHIPPING

Freight Classification: Rubber Accelerators or Softeners NOIBN. Parcel post, air express, air freight allowed.

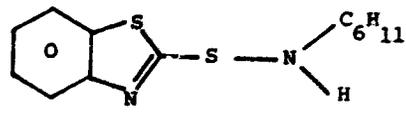
HANDLING

Material Safety Data Sheet available on request.

1/1/83

EFFECTS INFORMATION PROFILE

Aug 16 1983

ID No. 36	CHEMICAL NAME 2-Benzothiazole sulfenamide N-cyclohexyl	SYNONYMS Benzothiazyl 2-cyclohexylsulfenamide <i>Santipur CBS-</i>	CAS No. 95-33-0			
Description Cream colored powder		Use Rubber accelerator				
Melting point: 93-100°C Vapor pressure (B.P.): Specific gravity: 1.27 Water solubility: Insoluble Organic solubility: soluble in benzene Log P oct/water: 2.39 Empirical formula: C ₁₃ H ₁₆ N ₂ S ₂		Structural Formula 				
Biochemical Information			Observations in Humans			
<u>Reference</u>	<u>Nature of Info.</u> Pharmacology Anti Xa activity Hepatic cytochrome	<u>Page</u> 3-5	<table border="1"> <tr> <td data-bbox="787 903 998 1207"><u>Reference</u> Dekker & Reisma (1979)</td> <td data-bbox="998 903 1307 1207"><u>Nature of Info.</u> Duodenal ulcer</td> <td data-bbox="1307 903 1437 1207"><u>Page</u> 11</td> </tr> </table>	<u>Reference</u> Dekker & Reisma (1979)	<u>Nature of Info.</u> Duodenal ulcer	<u>Page</u> 11
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Toxicological Information			Environmental Information			
<u>Reference</u>	<u>Nature of Info.</u> Hygienic assessment Teratology - <i>positive</i> Mutagenicity - <i>negative</i>	<u>Page</u> 6-10	<table border="1"> <tr> <td data-bbox="787 1260 998 1543"><u>Reference</u></td> <td data-bbox="998 1260 1307 1543"><u>Nature of Info.</u> Ecology Microbial degradation</td> <td data-bbox="1307 1260 1437 1543"><u>Page</u> 12-15</td> </tr> </table>	<u>Reference</u>	<u>Nature of Info.</u> Ecology Microbial degradation	<u>Page</u> 12-15
<u>Reference</u>	<u>Nature of Info.</u> Ecology Microbial degradation	<u>Page</u> 12-15				
Enclosures			Page			
RTECS			2			

0051

RTECS

95 3 /C7
USER:
95-33-0 (R)
PROG:
13 (3) PST6 (1)

95 4 /C7
USER:
PRINT FULL COMPLETE INDENTED
PROG:

SECONDARY SOURCE ID
CAS TYPE 1 NAME
CAS REGISTRY NUMBER
STATUS
STATUS

MIDSH/DL6250006
2-BENZOTHIAZOLESULFENAMIDE; N-CYCLOHEXYL-
95-33-0
REPORTED IN EPA TSCA INVENTORY; 1980
MEETS CRITERIA FOR PROPOSED OSHA MEDICAL RECORDS RULE
FEREAC 47,30426,82

TOXIC DATA SOURCE

NTIS** NATIONAL TECHNICAL INFORMATION SERVICE;
PB223-159

TOX DATA KEYWORDS

ORAL; MOUSE; RODENTS; TDLO: 76 MG/KG/78W-1; TOXIC EFFECTS
EQUIVOCAL TUMORIGENIC AGENT

TOXIC DATA SOURCE

CSLNX* U. S. ARMY ARMAMENT RESEARCH & DEVELOPMENT
COMMAND; CHEMICAL SYSTEMS LABORATORY; NIOSH EXCHANGE
CHEMICALS; NX#02243

TOX DATA KEYWORDS

INTRAVENOUS; MOUSE; RODENTS; LD50: 32 MG/KG; TOXIC EFFECTS

BIOCHEMICAL INFORMATION

83

- SI - TOXBIB/83/146200
- AU - Mieriks J
- AU - Hesse W
- AU - Jaitly KD
- AU - Koekkoek PH
- AU - Lavy U
- AD - Gist-Brocades n.v. Research & Development, Delft, The Netherlands.
- TI - Pharmacological properties of colloidal bismuth subcitrate (CBS, DE-NOL).
- SO - Scand J Gastroenterol [Suppl]; VOL 80, 1982, P11-6
- LA - Eng
- CD - SJGSB
- IS - 0085-5928
- AB - ~~In pharmacological ulcer models in rats colloidal bismuth subcitrate (CBS) demonstrated anti-ulcer activity. This was neither a result of an acid neutralizing nor of an acid secretion inhibitory effect. Both in vitro and in vivo, an anti-peptic action was found. At low pH CBS precipitates and was shown to form a coating on the gastric wall especially on the ulcer crater. This coating most likely forms a protective barrier to the peptic activity of gastric juice. Low toxicity was seen following chronic daily administration of high doses of CBS for 3 months to rats and 6 months to dogs. Although the blood levels were more elevated in rats, the tissue bismuth levels were comparable in the two species (except for the caecum). The chief bismuth-excreting organs, the kidneys, showed relatively high concentrations, while the brain-concentrations were extremely low in concordance with the absence of nervous system toxicity.~~ *X Missing material*
- KW - TOXBIB
- KW - Animal
- KW - Anti-Ulcer Agents *PHARMACODYNAMICS ANTIULCER AGENTS
- KW - Bismuth METABOLISM/*PHARMACODYNAMICS
- KW - Chemistry
- KW - Colloids

BIOCHEMICAL INFORMATION

63

- BI - CA/098/137093A
- CC - CA/101001
- AU - Duthilleul P
- AU - Bouillet L
- AU - Fruchart JC
- AD - Dep. Lipides-Lipoproteines-Normolipemiants, Fac. Pharm. Lille, Lille

TI - Assay of the anti Xa activity of heparin: application of centrifugal analysis

SO - Clin. Chem. Newsl.; VOL 2, ISS June, 1982,91-5

PT - JOURNAL ARTICLE

CY - Fr.

ZP - 39000

LA - FRE

CD - CLNRD

AB - CBAC COPYRIGHT: CHEM ABS The anti-Xa activity of heparin [9005-49-6] was detd. in plasma of patients receiving heparin s.c. by an automated method with a centrifugal analyzer by using the chromogenic substrate CBS 3139 [83160-48-9], antithrombin III [9000-94-6], and blood platelet factor 4 [37270-94-3], and the results were compared to those obtained by other methods. The effect of the concns. of antithrombin III and platelet factor 4 on the method was examd. The relative std. deviations for repeatability and day-to-day reproducibility ranged 2.5-6 and 4.5-7.9%, resp. The detection limit was 0.02 units/mL, and there was a significant correlation between the results of the method and those obtained by chromometric methods. There was also good correlation between the anti-Xa and anti-IIa activities.

X Wrong material

RN - 9000-94-6; 9002-04-4; 9002-05-5; 9005-49-6; 37270-94-3; 83160-48-9

EM - 8305

CONTINUE PRINTING? (YES/NO)

0054

BIOCHEMICAL INFORMATION

CONTINUE PRINTING? (YES/NO)

USER:
YES
PROG:

16

X Wrong material

- SI - PESTAB/80/1421
 AU - Goldstein JA
 AU - Linko P
 AD - NIEHS, NIH, Research Triangle Park, NC 27709
 TI - Alteration of hepatic cytochrome P-450s by chlorinated benzenes (CBs).
 SO - Fed. Proc. Fed. Am. Soc. Exp. Biol. 39(3Pt2): 864 1980
 CD - FEPA
 AB - PESTAB. Rats were given high doses of CBs (250 mg/kg) po or in the diet [1000 ppm hexachlorobenzene (HCB)] for 1 wk. HCB increased benzpyrene hydroxylase (AHH) activity 16-fold, aminopyrine N-demethylase (ND) 3-fold, ethoxyresofurin O-de-ethylase (ERR) 42-fold, and cytochrome P-450 4-fold. The increase in ND resembles that produced by phenobarbital. The increases in AHH and ERR are much greater than those seen with phenobarbital (2.4-fold and 25%), but somewhat less than that produced by 3,4-benzpyrene (BP) (25- and 150-fold). The absorption maximum of the CO-difference spectrum of HCB induced microsomes (449 nm) is intermediate between that of phenobarbital (450 nm) and BP induced microsomes (448 nm). -Naphthoflavone selectively inhibited ERR activity in BP and HCB induced microsomes (94 and 88%) compared to control and phenobarbital induced microsomes (61 and 53%). In contrast to HCB, other CBs produced increases in cytochrome P-450, ND, AHH, and ERR similar to those produced by phenobarbital. The order of potency was 1,2,4-triCB > pentaCB > 1,2,3,5-tetraCB > 1,2,3,4-tetraCB > 1,3,5-triCB >> 1,4-diCB. Although the enzymatic properties of the cytochrome P-450 induced by HCB appeared similar to a mixture of phenobarbital and BP induced cytochromes, SDS polyacrylamide gel electrophoresis of the HCB induced microsomes indicated no increases in the two protein bands primarily increased by BP (with molecular wts of 55,000 and 57,000), but rather large increases at 50,000, 53,000 and 54,000. [Abstract 3149 of the annual meeting of the Fed. Am. Soc. Exp. Biol.] (Author abstract by permission)

RN - 118-74-1
 EM - 8005

CONTINUE PRINTING? (YES/NO)

0055

TOXICOLOGICAL INFORMATION

- 46
- SI - CA/098/08449BC
- CC - CA/104003
- AU - Korhonen A
- AU - Hemminki K
- AU - Vainio H
- AD - Dep. Ind. Hyg. Toxicol., Inst. Occup. Health, Helsinki
- TI - Embryotoxicity of benzothiazoles, benzenesulfohydrazide, and dithiodimorpholine to the chicken embryo
- SO - Arch. Environ. Contam. Toxicol.; VOL 11, ISS 6, 1982,753-9
- PT - JOURNAL ARTICLE
- CY - Finland
- ZP - SF-00290/29
- LA - ENG
- CD - AECTC
- IS - 0090-4341
- AB - CBAC COPYRIGHT: CHEM ABS Benzothiazole accelerators, 2-mercaptobenzimidazole [583-39-1], benzenesulfohydrazide [80-17-1], pentachloroethoxyphenol [133-49-3], a mixt. of alkylphenoldisulfides, alkylphenylformaldehyde resin, and 4,4'-dithiodimorpholine (I) [103-34-4], were tested on 3-day chicken embryos for toxicity. The parameters measured were early deaths, recorded within 2 days of injection, late deaths of malformed embryos, late deaths of nonmalformed embryos, and malformed survivors. The most embryotoxic of the chems. was I. Next in potency were N-tert-butyl-2-benzothiazylsulfenamide [95-31-8], N-oxydiethylene-2-benzothiazylsulfenamide [102-77-2], and benzenesulfohydrazide. ED50 values for total effect, including deaths and malformations, varied from 0.09 $\mu\text{mol/egg}$ to 2.6 $\mu\text{mol/egg}$ for these chems. I caused the highest frequencies of malformations.
- RN - 80-17-1; 95-31-8; 95-33-0; 102-77-2; 103-34-4; 133-49-3; 149-30-4; 583-39-1
- EM - 8304

95-31-8

No specific discussion of fox effects of 95-33-0

0056

TOXICOLOGICAL INFORMATION

Ex

- 26
- SI - ETIC/74/014886
- AU - KEPLINGER ML
- AU - FANCHER OE
- AU - LYMAN FL
- AU - CALANDRA JC
- TI - TOXICOLOGIC STUDIES OF FOUR FLUORESCENT WHITENING AGENTS
- SO - TOXICOL APPL PHARMACOL; 27:494-506,1974
- CD - TXAPA
- AB - ETIC/DRNL SEE: CA 81-86551
- KW - THALIDOMIDE
- KW - TINOPAL RBS
- KW - TINOPAL AMB
- KW - TINOPAL SBH
- KW - TINOPAL CBS
- KW - FLUORESCENT WHITENING AGENTS
- KW - MAMMAL, RABBIT
- KW - ORYCTOLAGUS
- KW - ALBINO

X *Wing material*

with active duodenal ulceration were randomly allocated either to treatment with CBS or to a placebo for a period of four weeks. Symptomatic assessment was based on frequency and severity of pain. The ulcer size was measured endoscopically before and at the end of the trial. During the trial blood and urinary bismuth concentrations were measured. The symptomatic assessment of the patients receiving CBS or placebo showed that the reduction in pain was highly significant in both groups, but there was statistically significant difference in the degree of reduction of duodenal ulcer size in favour of the colloidal bismuth subcitrate-treated group (p less than 0.025). Although a marked increase in urinary bismuth concentration was noted, the blood bismuth levels remained within the acceptable levels.

- KW - TOXBIB
- KW - Adult
- KW - Aged
- KW - Bismuth ADVERSE EFFECTS/METABOLISM/*THERAPEUTIC USE
- KW - Clinical Trials
- KW - Colloids
- KW - Double-Blind Method
- KW - Duodenal Ulcer *DRUG THERAPY/METABOLISM
- KW - Female
- KW - Human
- KW - Male
- KW - Middle Age
- KW - Placebos
- EM - 8001

0057

TOXICOLOGICAL INFORMATION

12
 BI - HECP/82/06734
 AU - STANKEVICH VV
 AU - VLASYUK NG
 AU - PROKOF'EVA LB
 TI - HYGIENIC ASSESSMENT OF ORGANIC SULFUR ACCELERATORS OF
 VULCANIZATION IN RUBBERS FOR THE FOOD INDUSTRY
 SO - BIO SANIT; 0 (10). 1980 (RECD. 1981). 88-89.
 LA - RUS
 CD - GISAA
 AB - HECP COPYRIGHT: BIOL ABS. NOTE RAT PROCESSING
 RN - 14634-93-6; 137-26-8; 103-34-4; 95-33-0
 EH - 8205

13
 BI - CA/096/137318H
 AU - ~~STANKEVICH VV~~
 AU - ~~VLASYUK NG~~
 AU - ~~PROKOF'EVA LB~~
 TI - ~~HYGIENIC ASSESSMENT OF ORGANIC SULFUR ACCELERATORS ON EMBRYONAL DEATH IN RATS~~
 SO - Byull. Eksp. Biol. Med.; VOL 93, ISS 1, 1982, 87-8
 PT - JOURNAL ARTICLE
 CY - USSR
 LA - RUS
 CD - BEBMA
 IS - 0365-9615
 AB - CBAC COPYRIGHT: CHEM ABS Investigated vulcanizers (VA) caused
 no significant intoxication changes in pregnant and nonpregnant
 rats. They affected the ovarian cycle when administered during
 the estrus. Altax (I) [120-78-5] prolonged the cycle the most,
 whereas santocure MDR [102-77-2] had the least effect. All the
 females showed a substantial redn. in the wt. of their
 offsprings. Administration of VA during pregnancy showed
 increased total embryo deaths but postimplantation lethality
 increased only following the administration of I and santocure
 [95-33-0]. All the VA reduced reprod. sharply.
 RN - 95-33-0; 97-77-8; 102-77-2; 120-78-5; 137-26-8; 149-30-4
 EH - 9205

CONTINUE PRINTING? (YES/NO) ✓

0 0 5 8

TOXICOLOGICAL INFORMATION

PROG:

SI - TOXPID/82/161353
 AU - Aleksandrov SE
 TI - [Effect of vulcanizing accelerants on embryoletality in rats]
 SO - Biull Eksp Biol Med; VOL 93, ISS 1. 1982, P87-8
 LA - Rus
 CD - BEBMA
 IS - 0006-4041
 AB - Embryonal lethality (EL) in rats was examined after administration of the rubber accelerators (RA), captax, altax, santocure, santocure-mor and thiurams D and E. Administration of RA to non-pregnant females caused the increase in the estrous cycle and diminished the rate of conception. The total EL increased after administering all the RA, while the postimplantation one only after altax administration. The index of altax mutagenicity is comparable with those of cancerogens or alkylating agents. Administration of RA to pregnant female leads to the increase in the total EL, with altax being the single agent that produces the rise in all the types of lethality. Inhibition of reproduction function of white rats is a consequence of mutagenic, embryotic and gonadotropic actions of RA, with altax being found the most active agent.

KW - TOXBIB
 KW - Animal
 KW - Comparative Study
 KW - English Abstract
 KW - Estrus DRUG EFFECTS
 KW - Female
 KW - Fetal Death *CHEMICALLY INDUCED
 KW - Mutagens *
 KW - Pregnancy
 KW - Rats
 KW - Thiazoles *TOXICITY
 KW - Thiocarbamates *TOXICITY
 KW - Thiram *TOXICITY
 KW - Time Factors
 RN - 120-78-5; 137-26-8; 149-30-4; 41365-24-6
 EM - 8207

CONTINUE PRINTING? (YES/NO)

USER:
 YES
 PROG:

0059

TOXICOLOGICAL INFORMATION

USER:
YES
PROG:

N. 5

SI - CA/098/084705T
 CC - CA/104006
 AU - You X
 AU - Zhou Y
 AU - Hu Y
 AD - Shanghai Inst. Ind. Hyg. Occup. Dis., Shanghai
 TI - Mutagenicity of fourteen rubber accelerators
 SD - Huanjing Kexue; VOL 3, ISS 6, 1982,39-42
 PT - JOURNAL ARTICLE
 CY - Peop. Rep. China
 LA - CHI
 CD - HCKHD
 IS - 0250-3301
 AB - CBAC COPYRIGHT; CHEM ABS

The mutagenicity of 14 rubber accelerators was detd. by using Salmonella typhimurium TA100 or TA98 in the presence or absence of S-9 mixt. Tetramethyl thiuram monosulfide [97-74-5] Showed pos. reactions in TA100 and TA98 in the presence of S-9 mixt. Tetramethyl thiuram disulfide [137-26-8] Showed pos. reactions in TA100 in the presence or absence of S-9 mixt., and the mutagenicity in TA98 was greater in the presence than in the absence of S-9 mixt. Zn diethyldithiocarbamate [14324-55-1] Showed pos. results in TA100 and TA98 in the presence of S-9 mixt. Dithiobis(benzothiazole) [120-78-5] was a weak mutagen. Tetraethyl thiuram disulfide [97-77-8], dimercaptobenzothiazole [39050-77-6], 2-(4-morpholindithio)benzothiazole [95-32-91], N-cyclohexylbenzothiazole-2-sulfenamide [95-33-01], N,N-dicyclohexylbenzothiazole-2-sulfenamide [4979-32-2], N-(oxydiethylenebenzothiazole)-2-sulfenamide [102-77-2], N,N-diisopropylbenzothiazole-2-sulfenamide [95-29-4], N-tert-butylbenzothiazole-2-sulfenamide [95-31-8], And diphenvylguanidine [102-06-7] and NA-72 [96-45-7] were inactive.

OBSERVATIONS IN HUMANS

PRUG:

- 24
SI - TOXBIB/80/041097
AU - Dekker W
AU - Reisma K
AD - Department of Internal Medicine, St. Elisabeth's of Groote Gasthuis, Haarlem, The Netherlands. ✓
TI - Double-blind controlled trial with colloidal bismuth subcitrate in the treatment of symptomatic duodenal ulcers with special references to blood and urine bismuth levels.
SO - Ann Clin Res: VOL 11, ISS 3, 1979, P94-7
LA - Eng
CD - ACLRE
IC - 0003-4762
AB - ~~To test the efficacy and toxicity of colloidal bismuth subcitrate (CBS) in a double-blind trial, forty-six consecutive outpatients with active duodenal ulceration were randomly allocated either to treatment with CBS or to a placebo for a period of four weeks. Symptomatic assessment was based on frequency and severity of pain. The ulcer size was measured endoscopically before and at the end of the trial. During the trial blood and urinary bismuth concentrations were measured. The symptomatic assessment of the patients receiving CBS or placebo showed that the reduction in pain was highly significant in both groups, but there was statistically significant difference in the degree of reduction of duodenal ulcer size in favour of the colloidal bismuth subcitrate-treated group (p less than 0.025). Although a marked increase in urinary bismuth concentration was noted, the blood bismuth levels remained within the acceptable levels.~~ *X Wrong material!*
KW - TOXBIB
KW - Adult
KW - Aged
KW - Bismuth ADVERSE EFFECTS/METABOLISM/*THERAPEUTIC USE
KW - Clinical Trials
KW - Colloids
KW - Double-Blind Method
KW - Duodenal Ulcer *DRUG THERAPY/METABOLISM
KW - Female
KW - Human
KW - Male
KW - Middle Age
KW - Placebos
EM - B001

ENVIRONMENTAL INFORMATION

2

SI - HEEP/83/07146

AU - SCHOCKEN MJ

AU - SPEEDIE MK

AU - KIRK P W JR

AD - Dep. Medicinal Chem./Pharmacognosy, Univ. Maryland Baltimore, 636
West Lombard St., Baltimore, MD 21201.

TI - Interaction of higher marine fungi with the herbicide atrazine:
1. Survey of interactive modes.

SO - MYCOLOGIA; 74 (5). 1982. 801-808.

CD - MYCOA

AB - HEEP COPYRIGHT: BIOL ABS. Eight species of marine Ascomycetes
and Deuteromycetes (*Ceriosporopsis halima* Linder (R-552),
Leptosphaeria oraemaris Linder (R-697), *Lulworthia* sp. (ATCC
36312), *Dendryphiella salina* (Suth.) Pugh et Nicot (CBS 142.60),
Monodictys pelagica (Johnson) Jones (F-80), *Periconia prolifica*
Anastasiou (F-109), *Trichocladium achrasporum* (Meyers et Moore)
Dixon (F-92) and *Zalerion maritimum* (Linder) Anastasiou (F-94))
indigenous to the Chesapeake Bay (USA) were surveyed for their
ability to interact with the herbicide atrazine. In liquid shake
cultures of artificial seawater containing glucose and NH_4NO_3 ,
the fungi mediated losses of atrazine ranging from 8-18% of 30
ppm and 9-68% of 500 ppm. Adsorption to the cell surface was
generally a minor component of loss at the lower concentration.
L. oraemaris grew with 500 ppm of purified atrazine as the sole
exogenous source of C or N, but not of both nutrients, and *P.*
prolifica had statistically significant growth compared to
controls when atrazine was the sole exogenous N source.
Apparently, filamentous marine fungi contribute to the
bioaccumulation and biodegradation of atrazine in estuaries.

wrong material

X

RN - 1912-24-9

EM - 8306

0062

ENVIRONMENTAL INFORMATION

USER:
YES
PROG:

F.V.
14

SI - CA/096/081319T
 CC - CA/10500e
 AU - Zeyer J
 AU - Bodmer J
 AU - Huetter R
 AD - Mikrobiol. Inst., ETH-Zurich, Zurich
 TI - Microbial degradation of ammeline
 SO - Zentralbl. Bakteriolog., Mikrobiol. Hyg., Abt. 1, Orig. C; VOL 2,
 ISS 3, 1981,289-98
 PT - JOURNAL ARTICLE
 CY - Switz.
 ZP - B092
 LA - ENG
 CD - ZBMMD
 AB - CBAC COPYRIGHT: CHEM ABS The biodegrdn. of ammelidine (I) [645-92-1], common product of the microbial degrdn. of s-triazine herbicides, was investigated using 165 microbial strains. Of all strains tested, 95% were able to degrade I to ammelide [645-93-2] and 35% could degrade ammelide further to cyanuric acid [108-80-5] which was accumulated in the growth medium. Only strain CBS 472.48 of Sporothrix schenckii was capable of metabolizing I slowly to CO₂ and NH₄⁺. The highest specific rate for I degraded to cyanuric acid was 3.3 μ kat (mol/s) .times. kg dry wt. of cells⁻¹. The deamination of I was usually the rate-limiting step. The enzymes degrading I to cyanuric acid were formed constitutively. NH₄⁺ and urea, however, caused repression of enzyme synthesis, and NH₄⁺ caused a slight inhibition of the I-degrading enzyme activity. Efficient degrdn. of I to CO₂ and NH₄ (0.4 μ kat .times. kg dry wt. of cells) could be achieved using a mixed culture of a pseudomonad, strain 123B, and S. schenckii strain 6.2.

RN - 108-80-5; 645-92-1; 645-93-2
 EM - B204
 CONTINUE PRINTING? (YES/NO)

X Wrong material

USER:
YES
2222.

ENVIRONMENTAL INFORMATION

USER:
YES
PROG:

J
17

- SI - PESTAB/80/1355
- AU - Keenemann H
- AU - van Leeuwen K
- AD - Dep. Vet. Pharmacol. & Toxicol., Univ. Utrecht, NL-3572 BP
Utrecht, The Netherlands
- TI - Toxicokinetics in fish: accumulation and elimination of six
chlorobenzenes by guppies.
- SO - Chemosphere 9(1): 3-19 1980 (18 References)
- CD - CMSHA
- AB - PESTAB. Female guppies (*Poecilia reticulata*) were exposed to a
standardized mixture of six chlorobenzenes (CBs):
1,4-dichlorobenzene (p-dichlorobenzene; 160 ng/ml),
1,2,3-trichlorobenzene (100 ng/ml), 1,3,5-trichlorobenzene (100
ng/ml), 1,2,3,5-tetrachlorobenzene (40 ng/ml), pentachlorobenzene
(8 ng/ml), and hexachlorobenzene (4 ng/ml). After 19 days of
exposure the fish were removed to fresh water and elimination of
CBs was studied for 9 wk. At various intervals water samples and
individual fish were analyzed for CBs by gas chromatography with
a ⁶³Ni electron capture detector. A 2-compartment model was used
to describe the kinetics of the CBs. Uptake and elimination rate
constants and bioaccumulation were determined and correlated with
log P_{oct} (the partition coefficient of a substance between
n-octanol and water). Results indicate that a parabolic curve,
with an optimum at log P_{oct} = 5.4, is apparently a better
description of the relation of the uptake rate constant with log
P_{oct} than a straight line. Bioaccumulation increases with log
P_{oct}, until reaching an optimum value at log P_{oct} = 6.5.
- RN - 106-46-7; 12002-48-1; 118-74-1
- EM - 8005

Wrong
material

CONTINUE PRINTING? (YES/NO)

USER:



0064

ENVIRONMENTAL INFORMATION

FROM:

E: 15

- SI - CA/095/198186T
- AU - Van Klengeren B
- AD - Natl. Inst. Public Health, Bilthoven
- TI - An in vitro comparison of new cephalosporins with special reference to *Pseudomonas aeruginosa*
- SO - J. Antimicrob. Chemother.; VOL 8, ISS Suppl. B, 1981, 1-105
- LA - ENG
- CD - JACHD

Wong
M. H. H. H.
X

AB - CBAC COPYRIGHT: CHEM ABS Min. inhibitory concns. of cefoperazone, cefotaxime(I), ceftazidime, and moxalactam were detd. for staphylococci, Enterobacteriaceae, Haemophilus influenzae, and *Neisseria gonorrhoeae*. (62893-19-0 Cefoperazone)(63527-52-6 Cefotaxime)(72558-82-8 Ceftazidime)(64952-97-2 Moxalactam) The new compds. were 10-100-fold more active in vitro against Enterobacteriaceae and *H. influenzae* (including penicillinase-producing strains) than were the older cephalosporins. Against *N. gonorrhoeae*, including penicillinase-producing strains, I appeared to be the most active compd. (min. inhibitory concn. 0.002 mg/L), whereas the other new cephalosporins were approx. as active as cefuroxime. (55268-75-2 Cefuroxime) Cefoperazone, I, cefsulodin, ceftazidime, ceftriaxone Na, and moxalactam were tested against carbenicillin-susceptible (CbS) and carbenicillin-resistant (CbR) strains of *P. aeruginosa*. (52152-93-9 Cefsulodin)(74578-69-1 ceftriaxone Na)(4697-36-3 Carbenicillin) Against CbS strains the lowest min. inhibitory concn. values were obtained with ceftazidime (1 mg/L), followed by cefsulodin (1-2 mg/L), cefoperazone (2-4 mg/L), ceftriaxone (4 mg/L), moxalactam (4-8 mg/L), and I (8-16 mg/L). Usually the susceptibility to cephalosporins of CbR strains was decreased for all compds., but this effect was smallest for ceftazidime. Considerable cross resistance with carbenicillin was noted for cefsulodin and cefoperazone only. Lysates of 19 CbR strains have been screened for the presence of constitutive beta-lactamase. (9073-60-3 .beta.-Lactamase) Three enzyme types were found: pi 5.4 (n = 8), pi 5.3 (n = 5), and pi 5.7 (n = 6).

RN - 62893 19-0; 63527-52-6; 72558-82-8; 64952-97-2; 55268-75-2; 52152-93-9; 74578-69-1; 4697-36-3; 9073-60-3; 61-33-6; 153-61-7;



2,2'Dithiobisbenzothiazole
(CAS: 120-78-5)

Contains No CBI

Product Literature

Attached are copies of a Technical Data Sheet and Material Safety Data Sheet for PENNAC® MBTS - Pennwalt's product name for 2,2'Dithio-bisbenzothiazole (MBTS).

Annual Production Data and Trends

Confidential Business Information (CBI)
See enclosed envelope marked "TSCA-CBI".

Production Worker Exposure

Pennwalt has no domestic in-plant exposure for MBTS since the material is imported already bagged for domestic sale.

Product Use Exposure

Pennwalt is not familiar with personnel exposure during use of this material in the rubber manufacturing process. This exposure information is probably best determined through representatives of the rubber manufacturing industry. Occasional exposure to this material will occur, however, when bags are accidentally broken in transit or in the warehouses.

MBTS is consumed by reaction mechanisms during normal processing in the manufacture of rubber. Therefore, human exposure to this material following the rubber manufacturing process is not anticipated.

Environmental Exposure

MBTS is unlikely to have any significant environmental impact because it is consumed through reaction mechanisms during its use in the rubber manufacturing process.

The most likely routes of entry to the environment are through spillage or breakage, which are not predictable, and residue in bags. The bag residue, if not consumed during disposal by incineration, would amount to less than 1000 lbs. per 200,000 lbs. of starting material per year, assuming that 4 oz. is left in each bag.

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JUL 14 AM 9:16

2,2'Dithiobisbenzothiazole

(CAS: 120-78-5)

Page 2



Toxicological Data

Pennwalt does not possess any internally generated toxicity data for MBTS. The acute oral data (non-lethal to rats at 7.94 gm/kg) and acute dermal data (non-lethal to rabbits at 7.94 gm/kg) as shown on the attached MSDS suggest a relatively low order of acute toxicity.

0 0 6 7

Emergency Information

MATERIAL SAFETY DATA SHEET

"ESSENTIALLY SIMILAR" TO OSHA FORM 20
FORM 4500 (Rev. 9-88)

ADDRESS: Pennwalt Corporation

Three Parkway
Philadelphia, PA 19102

Pennwalt Product Name

Pennac MBTS

Pennwalt Code No.

0632

Chemical Name and Molecular Formula

Benzothiazole, 2,2'-dithio-



Emergency Phone Number(s)

Business: **215/587-7550**

Other: **313/285-9200**

CAS No.(s)

120-78-5 plus 149-30-4

Synonyms

2,2-Dibenzothiazyl Disulfide

Chemical Family

Aryl Cyclic Sulfide Disulfide

MATERIALS OR COMPONENTS	% w/w	HAZARD DATA (TLV, LD50, LC50, etc.)
2,2-Dibenzothiazyl Disulfide	94	See toxicity section
2-Mercaptobenzothiazole	min. 1.5 max.	

Packages:

Multiwall Paper Bag, 50 lbs. net

Rubber Accelerators or Softeners, NOIBN

Fiber Drum, 175 lbs. net

Boiling Point/Range °C	°F	Melting Point °C	°F	Freezing Point °C	°F	Molecular Weight (Calculated)
		170	338			332.2
Specific Gravity (H ₂ O=1)	@	°C	@	°C	°F	Vapor Density (Air=1)
1.54		25/25				
Solubility in H ₂ O	% Volatiles by Volume		Evaporation Rate		<input type="checkbox"/> Ether = 1 <input type="checkbox"/> Water = 1 <input type="checkbox"/> Butylacetate = 1	
negligible	0.5 max.					
Appearance and Odor	Other					
Cream to off-white powder.						

Flash Point °C	°F	Test Method	Flammable Limits Lower	% Upper	%	Autoignition Temperature/Fire Point °C	°F
Nonflammable							

EXTINGUISHING MEDIA
 Water-spray Water-fog Water stream CO₂ Dry chemical Alcohol foam Foam Earth or sand

SPECIAL FIRE FIGHTING PROCEDURES
 Do not enter building Allow fire to burn Water may cause frothing Do not use water

UNUSUAL FIRE AND EXPLOSION HAZARDS
 Dust explosion hazard Sensitive to shock Contamination Temperature Other (specify): **If involved in fire, sulfur dioxide is a product of combustion.**

STABILITY
 Stable Unstable
 CONDITIONS CONTRIBUTING TO INSTABILITY
 Thermal decomposition Photo degradation Polymerization Contamination

INCOMPATIBILITY - Avoid contact with
 Strong acids Strong alkalis Strong oxidizers Other (specify):

HAZARDOUS DECOMPOSITION PRODUCTS - THERMAL AND OTHER (list)
CO, CO₂, NO_x, SO₂

CONDITIONS TO AVOID
 Heat Open flames Sparks Ignition sources Other (specify):

STEPS TO BE TAKEN IF MATERIAL IS RELEASED OR SPILLED
 Flush with water Absorb with sand or inert material Neutralize Sweep or scoop up and remove Keep upwind. Evacuate enclosed spaces. Prevent spread or spill
 Dispose of immediately Other (specify):

WASTE DISPOSAL METHOD - Consult federal, state, or local authorities for proper disposal procedures.

CONTINUED ON REVERSE SIDE

NA - Not Applicable.

Before using product, read and follow directions and precautions on product label and literature.

Oral (acute)
non-lethal at 7.94 gm/kg (rats)

Dermal (acute)
non-lethal at 7.94 gm/kg (rabbits)

Eye
essentially non-irritating

Inhalation (acute)
Dust may cause discomfort.

Chronic, Subchronic, etc.

HEALTH HAZARD INFORMATION
 (continued from Page 1)

PERMISSIBLE EXPOSURE LIMIT (Specify if TLV/TWA or Ceiling [c])
 ACGIH 19 ___ OSHA 19 ___ Other: **not established**

IRRITATION
 Skin Severe Moderate
 Eye Severe Moderate Mild (transient)

CORROSIVITY
 Skin 4 hrs. (DOT) 24 hrs. (CPSC)
 Eye May cause blindness

SENSITIZATION
 Skin Respiratory Allergen

INHALATION EFFECTS
 Narcotic effect Cyanosis Asphyxiant

LUNG EFFECTS (Specify):

OTHER (Specify):
 Repeated contact - skin defatter Other (Specify):

INGESTION
 Induce vomiting Do NOT induce vomiting Give plenty of water Get medical attention Other (specify):

DERMAL
 Flush with soap and water Get medical attention Contaminated clothing - remove & launder Contaminated shoes - destroy Other (specify):

EYE CONTACT
 Flush with plenty of water for at least 15 minutes Get medical attention Other (specify):

INHALATION
 Remove to fresh air If not breathing, give artificial respiration Give oxygen Get medical attention Other (specify):

SPECIAL PROTECTION INFORMATION

VENTILATION REQUIREMENTS - Always maintain exposure below permissible exposure limits
 Consult an industrial hygienist or environmental health specialist Local exhaust Use with adequate ventilation Check for air contaminant and oxygen deficiency

Other (specify):

EYE
 Safety glasses Face shield Goggles

HAND (GLOVE TYPE)
 Polyvinyl chloride Neoprene Butyl rubber Polyvinyl alcohol Other (specify):
 Natural rubber Polyethylene

RESPIRATOR TYPE - Use only NIOSH / MESA approved equipment
 Self-contained Supplied air Can or cartridge gas or vapor Filter - dust Other (specify):

OTHER PROTECTIVE EQUIPMENT
 Rubber boots Apron Other (specify):

SPECIAL PRECAUTIONS

PRECAUTIONARY LABELING
 Wash thoroughly after handling Do not get in eyes, on skin or clothing Do not breathe dust Keep container closed Keep away from heat, sparks, and open flames Store in tightly closed containers

Do not store near combustibles Keep from contact with clothing and other combustible materials Empty container may contain hazardous residues Use explosion proof equipment Other (specify):

Other handling and storage conditions

Prepared by **Christie B. Johnson** Date **11/18/80** Address **3 Parkway, Phila., PA 19102** Phone **215/587-7550**

PLEASE NOTE ▶ "The above information is accurate to the best of our knowledge. However, since data, safety standards, and government regulations are subject to change and the conditions of handling and use, or misuse are beyond our control, Penwalt MAKES NO WARRANTY, EITHER EXPRESS OR IMPLIED, WITH RESPECT TO THE COMPLETENESS OR CONTINUING ACCURACY OF THE INFORMATION CONTAINED HEREIN AND DISCLAIMS ALL LIABILITY FOR RELIANCE THEREON. User should satisfy himself that he has all current data relevant to his particular use.

0 0 6 7



Dicumyl Peroxide
(CAS: 80-43-3)

Contains No CBI

Product Literature

Enclosed please find toxicity data, reports of health effects testing, and copies of our technical bulletins and Material Safety Data Sheets.

Annual Production Data and Trends

Confidential Business Information (CBI).
See enclosed envelope marked "TSCA-CBI".

Production Worker Exposure

Confidential Business Information (CBI)
See envelope marked "TSCA-CBI".

Product Use Exposure

Dicumyl peroxide is transported primarily in Liqua-Bin containers. These containers are commonly referred to as Intermediate Bulk Containers. They are manufactured of stainless steel and contain approximately 455 gallons (3500 pounds) of dicumyl peroxide. These containers are closed for transport and, therefore, exposure would only result from accidental release of the compound. This material is also sold in various formulations with inert solid excipients. Again, these containers are sealed for transport and, therefore, exposure would be limited to accidental release. In use these products are transferred either mechanically, in the case of a liquid, or manually, in the case of the compounded formulations. Again, the very low toxicity of this material leads us to believe that no significant risk to the worker using this material is presented. These compounds are consumed in the reaction processes in which they are used and, therefore, release from these processes is limited only to accidental releases.

Environmental Exposure

Dicumyl peroxide is manufactured in an open system with no specific controls to limit or eliminate release of the product to the environment. At present there are no acceptable or available sampling methods to detect the level of this peroxide in the air. The very low vapor pressure of dicumyl peroxide suggests a nonsignificant level of air contamination.

RECEIVED
OPPT/CBIC
94 JUL 14 AM 9:16



Environmental Exposure - Continued

Liquid waste from the production process is transported by underground pipeline to our wastewater treatment facility. There it is mixed with other plant liquid wastes in an equalization lagoon. The mixture is neutralized and subjected to biological degradation in an aeration tank. Solids are then separated in a clarifier and the effluent, after filtration, is discharged to the Genesee River. The waste treatment facility is operated in accordance with applicable New York State permits. On three different occasions, plant effluent sampling was analyzed for dicumyl peroxide. The maximum concentration of dicumyl peroxide obtained was 398.1 ppb.

Toxicological Data

The published values for the oral LD₅₀, 4.1 g/kg (rat) and dermal irritation, mild with no sensitization (human) suggest a relatively low order of acute toxicity.



MATERIAL SAFETY DATA SHEET
"ESSENTIALLY SIMILAR" TO OSHA FORM 20
FORM 4840 (Rev. 9-86)

ADDRESS: Pennwalt Corporation

Lucidol Division
1740 Military Road
Buffalo, NY 14240

IDENTIFICATION

Pennwalt Product Name
Luperox 500 R

Pennwalt Code No.
801

Chemical Name and Molecular Formula
Peroxide, bis(1-methyl-1-phenylethyl)
C₁₈H₂₂O₂

Synonyms
Dicumyl Peroxide - Recrystallized

Emergency Phone Number(s)
Business: **716/877-1740**
Other:

CAS No.(s)
80-43-3

Chemical Family
Dialkyl Peroxide

HAZARDOUS INGREDIENTS

MATERIALS OR COMPONENTS	% w/w
Dicumyl Peroxide	99.0 min.

HAZARD DATA (TLV, LD50, LC50, etc.)

See toxicity section.

SHIPPING INFORMATION

DOT SHIPPING NAME - Dicumyl Peroxide, Dry (For samples add: Ltd. Quantity)
FREIGHT CLASSIFICATION - Chemicals NOIBN
HAZARDOUS CLASSIFICATION - Organic Peroxide
IMCO PAGE NO. #5164 UN NO. #2121

PHYSICAL PROPERTIES

Boiling Point/Range: °C 38 °C 100°F °C °F
Melt: g Point: °C °F
Freezing Point: °C °F
Molecular Weight (calculated): 270.4

Specific Gravity (H₂O=1): 1.001 @ 40/40 °C
Vapor Pressure (mm Hg): °C °F
Vapor Density (Air=1):

Solubility in H₂O: insoluble
% Volatiles by Volume: Evaporation Rate: Ether = 1 Water = 1 Butylacetate = 1

Appearance and Odor: Crystalline solid
Other:

USE AND STORAGE DATA

Flash Point: °C 200°F Test Method: SETA Flammable Limits: Lower % Upper %
Autoignition Temperature/Fire Point: °C °F

EXTINGUISHING MEDIA
 Water-spray Water-fog Water stream CO₂ Dry chemical Alcohol foam Foam Earth or sand

SPECIAL FIRE FIGHTING PROCEDURES
 Do not enter building Allow fire to burn Water may cause frothing Do not use water See *

UNUSUAL FIRE AND EXPLOSION HAZARDS

Dust explosion hazard Sensitive to shock Contamination Temperature Other (specify): Can decompose with force if confined in fire.

REACTIVITY DATA

STABILITY: Stable Unstable
CONDITIONS CONTRIBUTING TO INSTABILITY: Thermal decomposition Photo degradation Polymerization Contamination

INCOMPATIBILITY - Avoid contact with: Strong acids Strong alkalis Strong oxidizers Other (specify):

HAZARDOUS DECOMPOSITION PRODUCTS - THERMAL AND OTHER (list):
Decomposition products are flammable. Methane, Acetophenone & Cumyl Alcohol. May also contain phenols.

CONDITIONS TO AVOID: Heat Open flames Sparks Ignition sources Other (specify): Rapid decomposition may occur at temperatures above 190°F.

SPILL OR LEAK

STEPS TO BE TAKEN IF MATERIAL IS RELEASED OR SPILLED:
 Flush with water Absorb with sand or inert material Neutralize Sweep or scoop up and remove Keep upwind. Evacuate enclosed spaces. Prevent spread or spill

Dispose of immediately Other (specify): Vermiculite or perlite use non-sparking tools

WASTE DISPOSAL METHOD - Consult federal, state, or local authorities for proper disposal procedures.

*If large quantities involved, evacuate area and fight fire from safe distance. Cool surrounding material with water. Heavy smoke and objectionable odors may evolve if involved in fire.

CONTINUED ON REVERSE SIDE

NA - Not Applicable.

Oral (acute)
LD50: 4100 mg/kg (rats) (20% solution in corn oil)

Dermal (acute)
Mild irritant - human patch test

Eye
Mild conjunctivitis (rabbit)

Inhalation (acute)

Chronic, Subchronic, etc.

TOXICITY

PERMISSIBLE EXPOSURE LIMIT (Specify if TLV/TWA or Ceiling [C])
 ACGIH 19 OSHA 19 Other: **Not established**

IRRITATION
 Skin Severe Moderate
 Eye Severe Moderate Mild (transient)

CORROSIVITY
 Skin 4 hrs. (DOT) 24 hrs. (CPSC)
 Eye May cause blindness

SENSITIZATION
 Skin Respiratory Allergen Narcotic effect Cytotoxic Asphyxiant

INHALATION EFFECTS
 Skin Respiratory Allergen Narcotic effect Cytotoxic Asphyxiant

LUNG EFFECTS (Specify):

OTHER (Specify):
 Repeated contact-skin defatter Other (Specify):

INGESTION
 Induce vomiting Do NOT induce vomiting Give plenty of water Get medical attention Other (specify):

DERMAL
 Flush with soap and water Get medical attention Contaminated clothing - remove & launder Contaminated shoes - destroy Other (specify):

EYE CONTACT
 Flush with plenty of water for at least 15 minutes Get medical attention Other (specify):

INHALATION
 Remove to fresh air If not breathing, give artificial respiration Give oxygen Get medical attention Other (specify):

VENTILATION REQUIREMENTS - Always maintain exposure below permissible exposure limits:
 Consult an industrial hygienist or environmental health specialist Local exhaust Use with adequate ventilation Check for air contaminant and oxygen deficiency

OTHER (specify):

EYE
 Face shield Safety glasses Goggles

HAND PROTECTIVE TYPE)
 Butyl rubber Polyvinyl alcohol Other (specify):
 Polyvinyl chloride Neoprene Natural rubber Polyethylene

RESPIRATOR TYPE - Use only NIOSH / MESA approved equipment
 Self-contained Supplied air Can or cartridge gas or vapor Filter - dust, fume, mist Other (specify):

OTHER PROTECTIVE EQUIPMENT
 Rubber boots Apron Other (specify):

PRECAUTIONARY LABELING
 Wash thoroughly after handling Do not get in eyes, on skin or clothing Do not breathe dust, gas, mist, or vapors Keep container closed Keep away from heat, sparks, and open flames Store in tightly closed containers & direct in cool place

Do not store near combustibles Keep from contact with clothing and other combustible materials Empty container may contain hazardous residues Use explosion proof equipment Other sunlight (specify):

Other handling and storage conditions
Hazardous decomposition occurs at 243°F (120°C) or when contaminated with strongly acidic material.

SPECIAL PROTECTION INFORMATION

Prepared by **Dennis C. Cardino** Date **11/10/80** Address **1740 Military Road, Buffalo, NY 14240** Phone **716/877-1740**

PLEASE NOTE: The above information is accurate to the best of our knowledge. It is not intended to replace safety data sheets, standards, and government regulations are subject to change and the conditions of handling and use, or in its use beyond our control. Pennwalt makes no warranty, either express or implied, with respect to the completeness or continuing accuracy of the information contained herein and disclaims all liability for reliance thereon. User should satisfy himself that he has all current data available to his particular use.

2,5-Dimethyl-2,5-di(t-butylperoxy) hexane
CAS# 78-63-7

Test	Result	References
Acute Intraperitoneal Toxicity (mice) 90%	1700 mg/kg	W&T
Acute Oral Toxicity (rats)	LD ₅₀ >32 g/kg	FDRL - 59
Acute Dermal Toxicity (rabbits)	LD ₅₀ 4.1±1.3 gm/kg	FDRL - 59

2,5-Dimethyl-2,5-di(t-butylperoxy) hexyne-3
CAS# 1068-27-5

Test	Result	References
Acute Intraperitoneal Toxicity (mice) 90%	LC ₅₀ 1850 mg/kg	W&T
Primary Skin Irritation (rabbits) 90%	Not a skin irritant	IRDC-164-005

Dicumyl Peroxide
CAS# 80-43-3

Test	Result	References
Acute Oral Toxicity (rats) 96% (min)	LD ₅₀ 4100 mg/kg	H-ORC-204C
Acute Inhalation Toxicity (rats & rabbits) Dust from 40% on filler	8-90 mg/cu. m. (6 hrs.) no effect	H-ORC-204C
Eye Irritation (rabbits) (50% in corn oil)	Mild conjunctivitis	H-ORC-204C CA 73, 2117 (1970)
Skin Irritation & Sensitization (human) (patch test) (96% min)	Mild irritation - No sensitization	H-ORC-204C
Skin Sensitization (guinea pigs) (Intradermal injection) (96%)	No sensitization	H-ORC-204C
Mutagenicity Ames Test	Negative	Y&Y

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KEY TO REFERENCES

- ACGIH** American Conference of Governmental Industrial Hygienists. TLV Listing - 1981 Edition.
- ACC** Arco Chemical Company - Internal Reports.
- BJM** British J. Ind. Medicine 27, 11-12 (January 1970)
- B.P. 828** British Patent 1,040,828 - 9/1/66.
- CA** Chemical Abstracts.
- CIVO** Central Instituut voor Voedingsonderzoek TNO (CIVO), Zeist, Holland - Reports for Akzo Chemie.
- | | | | | | |
|--------|-----------|---------|-----------|--------|----------|
| R-4707 | June 1975 | R-5340 | Aug 1977 | R-5601 | Jan 1978 |
| R-9-76 | Sept 1976 | R-9-77 | Sept 1977 | R-5619 | Jan 1978 |
| R-5150 | Oct 1976 | R-5519 | Oct 1977 | R-5624 | Feb 1978 |
| R-5170 | Nov 1976 | R-11-77 | Nov 1977 | R-6-79 | Jun 1979 |
| R-5171 | Nov 1976 | R-5568 | Dec 1977 | R-6141 | Aug 1979 |
| R-5341 | May 1977 | R-5574 | Dec 1977 | R-6143 | Aug 1979 |
| | | R-5599 | Jan 1978 | R-6304 | Dec 1979 |
| | | | | R-6366 | Feb 1980 |
- F & S** Floyd, E.P., and Stokinger, H.E., Am. Ind. Hygiene Assoc. J. 19, No. 3, 205 (1958).
- FDRL-50** Food & Drug Research Laboratories Inc. N.Y.C. [Reports to R.T. Vanderbilt Co. Inc. dated Sept. 18 and Nov. 25, 1959.]
- FDRL** Food & Drug Research Laboratories Inc., Waverly, N.Y. [Report to Lucidol Division, Pennwalt Corporation.]
- FMC** Data supplied by letter dated April 17, 1972 from H.M. Castrantas. FMC Corporation to Organic Peroxide Producers Safety Division of S.P.I.
- HJK** H.J. Kuchle - Zbl. Arbeits Med. 8, 25 (1958)
- H-ORC-204C** Hercules Bulletin ORC-204C
- H-ORC-304B** Hercules Bulletin ORC-304B
- H-OP-524A** Hercules Bulletin OP-524A
- HEW-76** U.S. Department of Health, Education and Welfare. National Institute for Occupational Safety and Health "Registry of Toxic Effects of Chemical Substances - 1976 Edition".
- HYSAAV** Hygiene and Sanitation 29, 103 (January 1964) (English Translation of Gigena Sanitariya).
- IBT** Industrial Bio-Test Laboratories, Inc. of Northbrook, Ill. Reports to PPG Industries, Inc.
- | | | | |
|-----------|---------|-----------|---------|
| IBT-A341 | 9/16/71 | IBT-A8766 | 7/27/70 |
| IBT-A8559 | 7/15/70 | IBT-A8767 | 8/24/70 |
- IBT-H** Industrial Bio-Test Laboratories, Inc., Northbrook, Illinois. Reports to Hercules Incorporated.
- | | | | |
|--------|-------------------|--------|--------------------|
| 76-13A | December 20, 1976 | 76-13D | September 28, 1978 |
| 76-13B | November 3, 1976 | 77-21 | |
| 76-13C | December 15, 1976 | | |
- IHFA** Industrial Hygiene Foundation of America, Inc. Pittsburgh, Pa. Reported dated May-June 1961 to PPG Industries, for "The Acute Oral Toxicity of Pure Isopropyl Percarbonate".

KEY TO REFERENCES

(Continued)

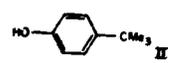
PPG-80D	PPG Industries, Inc. Bulletin 80-D 7/73
RTECS-79	"Registry of Toxic Effects of Chemical Substances" 1979 Edition (Published Sept. 1980) - U.S. Department of Health and Human Service, NIOSH. Also - Microfiche Edition - RETCS, Quarterly Issue, Oct. 1981 (Rec'd Feb. 1982)
SSE	Epstein, S.S. et al, <i>Toxicology & Applied Pharmacology</i> , 23, 288 (1972)
VLB	Van Duuren, B. L., et al., <i>J. Nat. Cancer Inst.</i> , 39, 1213 (1967)
VLG	Van Duuren, B. L., et al., <i>J. Nat. Cancer Inst.</i> , 39, 1217 (1967)
VLO	Van Duuren, B. L., et al., <i>J. Nat. Cancer Inst.</i> , 37, 825 (1966)
VON	Van Duuren, B. L., Orris, L. and Nelson, N., <i>J. Nat. Cancer Inst.</i> , 35, 707 (1965)
W.A.S.	Strong, W.A., <i>Ind. Eng. Chem.</i> , 56, No. 12,33 (1964)
W & T	Wallace & Tiernan, Inc. Belleville, N.J. Pharmaceutical Laboratory, Reports dated Feb. 1956 and Jan. 1960 to LUCIDOL DIVISION.
Y & Y	Yamaguchi, T. and Yamashita, Y., <i>Agricultural & Biological Chemistry</i> , 44 (7), 1965 (1980)

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[9001-00-0] activity in the liver, serum, and kidneys. It did not affect the enzyme activity in muscle.

97420a Comparative effect of low concentrations of di-tetra- and pentachloroethane on the blood acetylcholine system. Kuinskaya, I. L.; Verinskaya, R. V. (Ukr. Inst. Uprav. Vrach. Kharkov, USSR). *Gig. Tr. Prof. Zabol.* 1972, 10(6), 56-8 (Russ). In rabbits, exposure to 10 mg tetrachloroethane [79-34-5]/m³ for 3 hr/day 6 days a week for 7-8.5 months decreased blood acetylcholine [51-84-3] levels to a greater extent than did similar treatment with dichloroethane [1300-21-6] or pentachloroethane [76-01-7]. Acetylcholinesterase [9000-81-1] and butyrylcholinesterase [9001-00-5] activities of the blood were generally decreased by dichloroethane and pentachloroethane and were increased then decreased by tetrachloroethane.

97421p Metabolism of vitamin B₆ during occupational and common vitiligo. Galakhova, G. I.; Chumakov, N. N.; Spirichev, V. B. (Med. Sch., Yaroslavl, USSR). *Vop. Med. Khim.* 1972, 18(3), 296-301 (Russ). The blood vitamin B₆ (I)



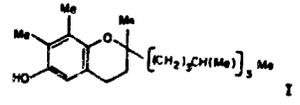
[8059-24-3] level was decreased 1.5-fold, while the urinary excretion of I and urea [57-13-6] remained normal in workers exposed to *p-tert-butylphenol* (II) [98-54-4] during the manufacture of phenolformaldehyde resins. These workers showed a 1.5-fold decrease in the urinary excretion of pyridoxinic acid [82-82-6] and a 3-4-fold increase in xanthurenic acid [59-00-7] excretion after tryptophan [73-22-3] loading. These metabolic disturbances were seen in exposed subjects whether or not the clin. symptoms of chem. vitiligo were present. In subjects with common vitiligo, but without exposure to II, no changes in I metabolism were seen. The effects of II were reversed by therapy with I.

97422q Activity of nucleases in rabbit lungs after inhalation of plutonium. Mushkacheva, G. S. (Inst. Biophys., Moscow, USSR). *Vop. Med. Khim.* 1972, 18(3), 301-5 (Russ). Following the inhalation of 1.5 μCi plutonium [7410-07-5] by rabbits, the acid DNase [9001-98-9] activity of lung tissue increased up to 139% of control during the 1st 2 weeks and up to 185% of control within the 1st month. Lung tissue acid RNase [9001-99-1] increased to 106-173% of control during the 4 months observation, while alk. RNase increased to 183% within the 1st month. The importance of nuclease activation during irradiation and post-irradn. recovery is discussed.

97423r Effect of carbon tetrachloride intoxication on the activity of multiple forms of esterases from serum and liver of rats. Surinov, B. P.; Bochkova, D. N.; Kashkin, K. P. (Res. Inst. Med. Radiol., Obninsk, USSR). *Vop. Med. Khim.* 1972, 18(3), 309-15 (Russ). Carbon tetrachloride [56-23-5], injected s.c. into rats, decreased the activities of aryl-, acetyl-, and carboxy-esterases in serum and liver. The liver ext., prepd. from CCl₄-treated rats and contg. deoxycholate, contained many esterase iso-forms which were not detected in the intact animals. The iso-forms could not be detected within 3 days after intoxication, although some reappeared within 10 days after intoxication.

97424s Experimental indium poisoning. Yoshikawa, Hiroshi; Hasegawa, Takeshi (Natl. Inst. Ind. Health, Kawasaki, Japan). *Igaku To Seibutsugaku* 1971, 63(2), 45-8 (Japan). Aq. indium sulfate [13464-82-9] (0.1-1.0 mg In/kg/day, s.c.) given to mice for 15 days caused marked anemia and damaged the lung, liver, and spleen. Pulmonary lesions were very marked. No subacute toxicity was obsd. with doses of 0.05 mg/kg. I. Matsumoto

97425t Ultrastructural changes of rat liver cells induced by yellow phosphorus. Kim, Sung Ho (Coll. Med., Yonsei Univ., Seoul, S. Korea). *Yonsei Uidae Nonmunjip* 1971, 4(2), 138-52 (Korean). Yellow phosphorus [7723-14-0] (0.75 mg/100 g, i.p.)

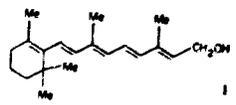


caused severe hepatic necrosis in rats, beginning with fatty metamorphosis by 6 hr after injection. In rats pretreated with *dl-γ-tocopherol* (I) [7540-59-2] (10 mg/100 g/day for 3 days), the fatty metamorphosis did not appear until the 12th hr after P injection and the pathol. effects of P were slightly decreased. In all cases, the fatty changes assocd. with P were not confined to the periphery of the hepatic lobules but involved the entire lobule even in the early stages. Since I did not completely prevent the toxic effects of P, the previously held lipoperoxidn. theory does not hold true for yellow P poisoning. Electron microscopic findings assocd. with the toxic effects of P on liver cells are

described in detail, the most significant finding being hyperphasic changes in the rough endoplasmic reticulum by 6 hr after P treatment.

97426u Toxicity of dietary ethionine and methionine to the pancreas and liver. Kim, Jae Joon (Coll. Med., Yonsei Univ., Seoul, S. Korea). *Yonsei Uidae Nonmunjip* 1971, 4(2), 168-82 (Korean). Rats fed low protein diets contg. 1% ethionine [67-21-0] for 6 weeks showed only slight toxic changes in the liver and pancreas, while rats fed 1% methionine [53-51-8] showed no toxic reactions in these organs. Rats fed ethionine showed wt. loss, a 33.3% mortality rate, destruction of pancreatic acini and liver cells, decreased serum amylase [9000-92-4] activity, and increased serum glutamic-oxalacetic transaminase [9000-97-9] and glutamic-pyruvic transaminase [9000-88-6] activities. Regeneration of the damaged tissues was seen beginning the 8th week of treatment with ethionine. In contrast, rats fed methionine showed wt. gain, 0% mortality, no damage to liver or pancreas, a slight increase in serum amylase activity, and no change in the transaminase activities.

97427v Ultrastructural changes of rat liver cells induced by large doses of vitamin A. Nam, Sang Hyok (Coll. Med., Yonsei Univ., Seoul, S. Korea). *Yonsei Uidae Nonmunjip* 1971, 4(2), 205-21 (Korean). Microscopic examn. of liver cells from



rats given 500 I.U. vitamin A (I) [11103-57-4]/g/d, γ showed mild fat droplet accumulation but no necrosis or balloon cells were seen. Livers from rats treated simultaneously with I and cortisone [53-06-5] (0.05 mg/g/day) showed balloon cells beginning on the 1st day and fat vacuolization beginning on the 10th day. Electron microscopic examn. of liver cells from I-treated rats showed dilation of the endoplasmic reticulum on the 3rd day, with localization of acid phosphatase [9001-77-8] outside of the intact lysosomes. Organelle and cytoplasmic damage was noted as time progressed. Thus, I facilitated enzyme leakage across the lysosomal membrane rather than membrane rupture. In rats treated with both I and cortisone, the release of acid phosphatase, the formation of lipids, and damage to the organelles were delayed.

97428w Effects of cadmium on the rat's teeth and on the compensating effects of chromium. Lee, Baeh Jhin (Coll. Med., Yonsei Univ., Seoul, S. Korea). *Yonsei Uidae Nonmunjip* 1971, 4(2), 255-64 (Korean). Cadmium chloride [10108-64-2] (0.1 mg/day for 14 days, orally) increased the serum Ca level, decreased the serum P level, increased the serum alk. phosphatase [9001-78-9] activity, decreased wt. gain, and caused preentin thickening and odontoblast atrophy in the anterior teeth. These effects were not seen in rats given both CdCl₂ and chromium trioxide [1333-82-6] (0.1 mg/day for 14 days). Rats liver and kidneys than rats given only CdCl₂ accumulated less Cd in the compensating action toward the effects of Cd.

97429x Sulfide inhibition of oxidases in rice roots. Allam, A. I.; Hollis, J. P. (Dep. Plant Pathol., Louisiana State Univ., Baton Rouge, La.). *Phytopathology* 1972, 62(6), 634-9 (Eng). Levels of hydrogen sulfide [7783-06-4] prevalent in the Louisiana rice fields during the heading-flowering stage inhibited the activities of cytochrome oxidase [9001-16-5], catalase [9001-05-2], peroxidase [9003-99-0], ascorbic acid oxidase [9029-44-1], and polyphenol oxidase [9002-10-2] in rice seedling roots in vitro. H₂S levels as low as 0.07-0.1 μg/ml significantly inhibited the respiration of rice seedling roots. Thus, redn. of rice root oxidative capacity, terminal oxidn., and other physiol. functions by H₂S may cause hitherto unrecognized toxic diseases of rice, manifested as reduced grain yields.

97430r Toxicity of organic lauroyl and dicumyl peroxides during a chronic experiment. Orlova, F. I. (USSR). *Sb. Nauch. Tr. Kuibyshev. Nauch.-Issled. Inst. Gig.* 1971, No. 6, 101-7 (Russ). From *Ref. Zh., Biol. Khim.* 1971, Abstr. No. 19F2119. Male rats were given dicumyl peroxide [80-43-3] and lauroyl peroxide [105-74-8] in doses equiv. to 0.02 or 0.004 LD₅₀ and I.D₅₀ with their food for 4 months. These prepra. decreased the Hb level and the amt. of erythrocytes, increased the reticulocytes in the peripheral blood, increased methemoglobin formation, decreased blood SH groups, and slightly decreased blood peroxidase activity. Total blood protein decreased due primarily to the drop in albumin fractions and a decreased synthesis of hippuric acid towards the end of the expt. Deta. of Hb and methemoglobin, erythrocytes and reticulocytes no., and the blood peroxidase activity are recommended for the early diagnosis of poisoning by these org. peroxides.

97431s Toxicological characteristics of dimethyldithiophosphoric acid. Aizenshtadt, V. S.; Perkhurov, V. P. (USSR).

(Se) Toxicity - Peroxides -

levels of available hepatic ATP to methionine, thereby forming increasing amounts of hepatocellular S-adenosylmethionine and S-adenosylhomocysteine. In support of the concept that the histone changes induced by methionine intoxication were mediated through a hepatic ATP isoenzyme was the finding that administration of 50 mg adenine sulfate to intoxicated animals completely reversed the hypoglycemic effects of methionine. The possibility that a similar mechanism of intoxication occurs in human methionine ingestion and hypermethionemic states is discussed.

2100v Hepatoprotective action of a natural polypeptide (PH-1) in experimental intoxication with carbon tetrachloride. Prejlo, Oh.; Timar, Magda; Todorova, M. (Inst. Ceret. Chim. Farm., Bucharest, Rom.). *Mofol. Norm. Patol.* 1969, 14(4), 217-22 (Rom.). The action of PH-1 polypeptide (I) (M. Timar, 1969) was tested for the treatment of acute, subacute, and chronic intoxication with CCl₄ in rats. It proved to be a hepatoprotective agent regarding the necrotic action of CCl₄, the restoration of hepatic metabolism, and the stimulation of regeneration. Liviu Vancea

2100w Cytotoxic and cancerostatic activity of isothiocyanates (ITC) and related compounds. V. ITC with sulfide and sulfone groups. Horakova, Katarina; Drobnica, Ludovit; Nemecek, Pavel; Uher, M. (Pac. Chem., Slovak Polytech. Univ., Bratislava, Czech.). *Neoplasm* 1970, 17(1), 3-8 (Eng.). Thirteen 4-isothiocyanatophenyl alkyl sulfones, and (4-substituted-4'-isothiocyanatodiphenyl) sulfones such as (4-isothiocyanatophenyl) Et sulfone (I) and (4-methyl-4'-isothiocyanatodiphenyl) sulfone and fourteen 4-isothiocyanatophenyl alkyl sulfides (4-substituted-4'-isothiocyanatodiphenyl) alkyl sulfides, such as (4-isothiocyanatophenyl) Me sulfide and (4-nitro-4'-isothiocyanatodiphenyl) sulfide, were synthesized and evaluated for cytotoxic and cancerostatic activities in HeLa cells. In general, isothiocyanate containing a sulfone group were more effective than those with a sulfide group. Among the 27 compounds tested, I was the most effective cytotoxic agent, while (4-dimethylamino-4'-isothiocyanatodiphenyl) sulfide was the least effective.

2100x Toxicity of PCP for the "Dojo" fish, *Misgurnis anguillicaudatus* with special reference to the relation between concentration and immersion time. Studies on the biological assay of chemicals in fishes. V. Nagasawa, Sumio; Michiyo, Shiba (Hara Agr. Chem. Inst., Shimizu, Japan). *Nippon Oyo Dobutsu Kenkyu Gakkaishi* 1969, 13(2), 47-51 (Japan). Dojo fish (10.4-12.7 g body wt.) were kept for 2 days in running water at 10°, dipped 50 min in 200 ml H₂O contg. 0.53-100 ppm of 90% pentachlorophenol Na salt (PCP), and returned again into the running water. The death probability (Y) could be represented by the regression curve; $Y = -5.1725 + 3.2485 \log C + 5.0678 \log T$, where C (ppm g) is PCP concn. per fish body wt. and T is the immersion time (min). The χ^2 test showed no significant difference between the empirical Y and that calc'd. from the regression curve.

2100y Toxic effects of dietary selenium in hamsters. Hadji-markos, Demetrios M. (Dent. Sch., Univ. of Oregon, Portland, Oreg.). *Nutr. Rep. Int.* 1970, 1(3), 175-9 (Eng.). The effects of chronic Se toxicity were studied in groups of weanling hamsters by the addn. to their drinking water of selenite-Se in the amounts of 6, 9, and 12 ppm. The results demonstrated that hamsters are far more resistant to Se toxicity compared with rats. The superior tolerance of hamsters to Se intake may find useful applications in areas of biomedical research which are concerned with the effects of long-term ingestion of Se on the organism.

2110a Biological effects of root canal filling materials. 5. Toxic effect in vitro of root canal filling materials on HeLa cells and human skin fibroblasts. Spangberg, Larz (Dep. Clin. Bacteriol., Univ. Umea, Umea, Swed.). *Odontol. Revy* 1969, 20(4), 427-30 (Eng.). Toxic effects of root canal filling materials, stabilized and emulsified by Tween 80 and in addn. filtered through a glass filter of pore size 1 μ were exam'd. In the individual materials, the following total inhibiting concns. for HeLa cells were found: N2 0.1, Riebler's paste 0.4, All 26 and Diaket 1.0, and Chlor-percha, Ca(OH)₂, Tubli-Seal and phosphate cement 0.4% (wt./vol.). Concns. of Ag. Gutta-percha, and Gutta-perch.: Osmicnicol up to 12.8% wt. vol. did not completely inhibit the growth of HeLa cells. The same order of the effect of the materials was found in human skin fibroblasts, though the total inhibiting concns. were mostly twice as high showing that the fibroblasts were less sensitive. Thus, by the removal of particles larger than 1 μ , the toxicity of suspensions decreased in comparison with the previous results. J. A. Ruzicka

2111t Effect of carbon disulfide on metabolism and visceral changes in experimental animals. V. Activity of aspartic aminotransferase, alanine aminotransferase, and malate dehydrogenase in serum and liver homogenate of rats chronically poisoned with intraperitoneally administered carbon disulfide. Groyowczyk, Janusz (Pomorska Akad. Med., Szczecin, Poland). *Patol. Pol.* 1970, 21(1), 85-91 (Pol.). In rats poisoned 100 days with CS₂ (20 mg/kg i.p. every other day), activity of the title enzymes in serum was essentially unchanged. In liver homog-

enates only malate dehydrogenase activity showed significant changes (from 229 to 276.24 units/mg protein N), which were attributed to liberation of the enzyme from the damaged mitochondria.

2112a Effect of carbon disulfide on metabolism and visceral changes in experimental animals. III. Morphological changes and behavior of acid and alkaline phosphatase and lipids in the liver of rats chronically poisoned by intraperitoneal administration of carbon disulfide. Glinka, Danuta; Kosmider, Kazimierz (Pomorska Akad. Med., Szczecin, Poland). *Patol. Pol.* 1969, 20(4), 397-405 (Pol.). Histochem. examn. of the liver of rats treated 60 or 120 days with CS₂ (25 mg/kg, i.p. every other day) revealed changes characteristic of liver damage. The changes were nonspecific and their intensity was proportional to the total CS₂ dose.

2113v Effect of vitamin C on ovaries and adrenals in stresses. Rokicki, Wladyslaw (Akad. Med., Cracow, Poland). *Patol. Pol.* 1969, 20(4), 455-9 (Pol.). In rats breathing furlural vapors for 7 months (0.132 mg/l. of air, 2 hr daily) a marked hypertrophy of adrenals and slight hypertrophy of ovaries were observed. The changes were more intense in animals which were forced to muscular effort at the time of poisoning. Vitamin C (100 mg daily i.p. for 7 days) administered to the animals of the latter group markedly reduced the hypertrophic changes. Prophylactic administration of vitamin C to workers exposed to furlural vapors was suggested.

2114w Toxicity and radioprophylactic action of 2-mercaptoethylguanidine and its derivatives in mice and in HeLa S₃ cells. Takagi, Yoshinari; Sato, Fumiko; Shikita, Mikio; Shinoda, Masato; Terashima, Toyozo; Akaboshi, Sanya (Nat. Inst. Radiol. Sci., Chiba, Japan). *Radiat. Res.* 1970, 42(1), 79-90 (Eng.). Introduction of a Me group(s) into N and (or) N' nitrogen of the guanido group of 2-mercaptoethylguanidine (MEG) significantly increased acute toxicity in mice of the mother compd. When compared on equimolar bases in some narrow ranges, N-methyl, N'-methyl, and N,N'-dimethyl derivs. showed a magnitude of prophylactic action against x-irradiat. in mice similar to MEG. However, the radioprophylactic range of these compds. was narrower than that of MEG. A deriv. having Me groups at N, N', and N'' was most toxic and no more radioprotective. Loss of reproductive integrity of x-irradiated HeLa S₃ cells was prevented by preincubation of the cells in a medium contg. 20-30 mM MEG. On the other hand, proliferation of cells was markedly inhibited by MEG itself, when the compd. was present in the medium for a long period even in a concn. as low as 0.1 mM. The derivs. of MEG also protected HeLa cells against x-rays, but to much less extent than MEG did. In addn., all these MEG derivs. were likewise less potent than MEG with respect to the inhibitory action on proliferation of HeLa cells.

2115x Toxicity of dimethyldioxane. Svechnikova, E. L.; Svirnova, L. V. (USSR). *Sb. Nauch. Tr. Kuibyshev. Nauch.-Issled. Inst. Epidemiol. Gig.* 1968, No. 5, 14-6 (Russ.). From *Ref. Zh., Farmakol., Khimioter. Sredstva, Toksikol.* 1969, Abstr. No. 5.54.670. The toxic effect of dimethyldioxane was measured by the Rosenthal-Savel'ov method. In rats, as in workers at synthetic rubber plants, a statistically significant decrease of propherlin titer in blood serum is observed. The propherlin titer detn. reaction is considered a sensitive test for early signs of dimethyldioxane intoxication.

2116y Toxicology of vat residues of tricresyl phosphate. Aizenstadt, V. S. (USSR). *Sb. Nauch. Tr. Kuibyshev. Nauch.-Issled. Inst. Epidemiol. Gig.* 1968, No. 5, 92-3 (Russ.). From *Ref. Zh., Farmakol., Khimioter. Sredstva, Toksikol.* 1969, Abstr. No. 5.54.635. In 3-week rat expts. it was shown that tricresyl phosphate vat residues (I) in a 5-10% NaHCO₃ soln. at 45° do not have absorption capability through skin that is intact. At the point of application in rats and rabbits, surface dermatitis, sometimes necrosis, was raised for 5-10 days. Within 3-4 days after applying 2 drops of I in 5% NaHCO₃ soln. to the eye, conjunctivitis developed. The LD₅₀ for mice (orally) was 1900-2000 mg/kg, and the max. tolerable dose was 500 mg/kg. Cumulative capability of I was insignificant. With daily internal doses of 0.4 mg/kg of I into rats, losses of wt. and work capability were noticed for 30 days, along with depression of cholinesterase activity in the blood. Its lack of skin absorptive properties, its low volatility, and its weak accumulative capability limit the effectiveness of I as a poison in industrial conditions. An effective medium for removing I from skin is a 3% NaHCO₃ soln.

2117z Toxicity of lauroyl and dicumyl peroxides. Orlova, F. T. (USSR). *Sb. Nauch. Tr. Kuibyshev. Nauch.-Issled. Inst. Epidemiol. Gig.* 1968, No. 5, 107-9 (Russ.). From *Ref. Zh., Farmakol., Khimioter. Sredstva, Toksikol.* 1969, Abstr. No. 5.54.654. Lauroyl peroxide (I) and dicumyl peroxide (II) are used as high-temp. polymn. catalysts in production of polystyrene plastics. The LD₅₀ of I given orally to mice was 10 g/kg. With oral application of 15 g/kg of II, 33% of the exptl. animals died. The minimally active dose of II orally was 1 g/kg. With a dose of 3 g/kg of II (orally), half of the exptl. rats died

within 10 days. At first the animals developed leukocytosis, which changed to leukopenia, and the Hb content in the blood was lowered. Within 2.53 months after treating the animals died with characteristics of anemia. A weak irritation reaction was noticed for 2 weeks after application of I and II on the skin. I and II in the rabbit eye induced the development of catarrhal conjunctivitis. **TRICH - MICE - MORW**

2118a Triethyl phosphate toxicity. Pyatlin, V. N. (USSR). *Sb. Nauch. Tr. Kazbyshev. Nauch.-Issled. Inst. Epidemiol. Gig. 1968, No. 5, 117-18 (Russ). From Ref. Zh., Farmakol., Khimioter. Sredstva, Toksikol. 1969, Abstr. No. 5.54.600. Mice were given triethyl phosphate orally; the LD₅₀ was 1370 (1250-1490) mg/kg. Poisoning was characterized by initial excitement followed by depression of the central nervous system, loss of movement coordination, paresis of rear extremities, breathing disordered, and lowering of muscle tonus. With daily oral administration of 1/5 LD₅₀ of triethyl phosphate, toxic effects were not apparent in the course of 1 month. Triethyl phosphate did not have an irritating effect with application to the skin of rabbits, and with entry into the eyes transient conjunctivitis appeared. A skin absorptive effect was not present. **MORW***

2119b Fatty acid profiles of cerebrospinal fluid lipids in normals and chronic alcoholics. Tichy, Jiri; Alling, Christer; Dencker, Sven J.; Svennerholm, Lars (Psychiat. Clin. II, Lillhagens Hosp., Goteborg, Swed.). *Scand. J. Clin. Lab. Invest. 1970, 25(2), 191-7 (Eng). Quant. detns. were made of the main lipid classes in cerebrospinal fluid (CSF) samples of normal males and of chronic alcoholics after acute abuse, and normal males and of chronic alcoholics after acute abuse, and normal males and of chronic alcoholics after acute abuse, and normal males and of chronic alcoholics after acute abuse. The fatty acid profiles of cholesteryl esters, triglycerides, and choline and ethanolamine phosphoglycerides were compared with those of corresponding serum samples. The most const. difference found between serum and CSF was the lower concn. of linoleic acid (18:2) in CSF, which was most pronounced for the 2 phosphoglycerides. The fatty acid profile of CSF from normals and alcoholics differed only regarding these two lipids. **RCCH***

2120v Alkaloids from catechol amines in adrenal tissue: possible role in alcoholism. Cohen, Gerald; Collins, Michael (Coll. of Phys. and Surg., Columbia Univ., New York, N.Y.). *Science 1970, 167(3926), 1749-51 (Eng). Epinephrine and norepinephrine condensed with AcHl or with HCHO (derivs. of BHOH metabolism) in dil. aq. soln. at neutral pH and room temp. to form 1,2,3,4-tetrahydroisoquinoline alkaloids. Similar condensation reactions occurred in cow adrenal glands; perular condensation reactions occurred at 37°. Biosynthesis of these alkaloids in vivo could play a role in altering an individual's behavior during and after the ingestion of alc. **RCMH***

2121w Effect of chronic intoxication with cadmium chloride on thermoregulation and glycemia in the white rat. Vinescu, Niculina; Chizelea, G.; Nersesian-Vasilii, Cornelia (Sect. Fiziol. Anim., Inst. Biol. "Traian Savulescu," Rom.). *Stud. Cercet. Biol., Ser. Zool. 1969, 21(6), 453-8 (Rom). The effect of small doses of CdCl₂ with prolonged activity was studied in rats. Administration of CdCl₂ in drinking water (3 mg Cd/animal during 235 days) in male or female rats arising from parents intoxicated for 10 months with the same doses of Cd, produced a disturbance of the chem. thermoregulation manifesting itself in a stimulation of the O consumption (rat, O consumption 1.4g/hr, body temp., temp. given): male rats, 1.280, 0.4° decrease, 20°; female rats, 1.762, —, 20°; male rats, 1.100, 37.2°, 30°; female rats, 1.120, 37.6°, 30°; male rats (control), 1.164, —, 20°; male and female rats (controls), 0.708-0.743, —, 30° (the normal body temp. of male and female rats being 36.6-37.2° before the expt.). CdCl₂ produced an increased glycemia (135, 115 as compared to 108, 103 mg/100 ml blood, for male and female rats, resp.). **Liviu Vancea***

2122x Adrenal morphology and histochemistry after administering alloxan to rats. Sucer, A.; Bratianu, Alice; Stroia, Veronica; Hescovici, B. (Lab. Fiziolopatol., Inst. Med. Farm., Iasi, Rom.). *Stud. Cercet. Embriol. Ciol., Ser. Ciol. 1969, 6(2), 160-75 (Rom). The effects of the i.m. administration of 100 or 200 mg alloxan/kg to rats were studied. Adrenal wt. was reduced to a min. after 12 hr. With the lower dose, wt. returned to normal after 72 hr, while the higher dose nearly doubled the wt. The drug caused significant modifications of adrenocortical structure, including degeneration. **Liviu Vancea***

2123y Acetonitrile and toxic emphysema. Arbuzov, E. E. (USSR). *Toksikol. Gig. Prod. Neftekhim. Neftekhim. Proizvod. 1968, 16-18 (Russ). From Ref. Zh., Farmakol., Khimioter. Sredstva, Toksikol. 1969, Abstr. No. 5.54.873. In rats, the LD₅₀ of acetonitrile, orally and s.c., is 3.6 g/kg; intraperitoneally, it is 0.92 g/kg. Injection of urethane, barbital, and chloral hydrate before or after acetonitrile poisoning sharply aggravates the course of intoxication, raising the coeff. of emphysema to 12.3-13 (9.7-9.8 with acetonitrile alone). Serotonin increases longevity of acetonitrile-poisoned rats, and with repeated injection decreases the coeff. of emphysema to 9.5. Aminazine, hexonim, and tropazine prevent development of emphysema. Daily injections of aminazine aids pulmonary development and sharply raises acetonitrile toxicity. **Acetonitril***

induce damage to the brain stem, autonomic ganglia, and receptors of the lung vessels. **MORW**

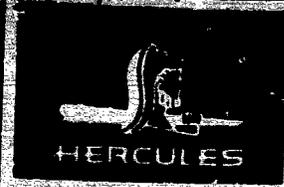
2124z Toxicology of some synthetic fat substitutes. Bykov, L. A. (USSR). *Toksikol. Gig. Prod. Neftekhim. Neftekhim. Proizvod. 1968, 25-9 (Russ). From Ref. Zh., Khim. 1969, Abstr. No. 111448. The toxic characteristics of synthetic C₁₈-C₂₄ fat substitutes were studied in animals before and after the removal of impurities (iso- and ketodicarboxylic acids). The toxicities were moderate. **NBRK***

2125a Toxicology of methylethylpyridine-HCl and dimethylpyridine-HCl. Makho, A. S. (USSR). *Toksikol. Gig. Prod. Neftekhim. Neftekhim. Proizvod. 1968, 78-80 (Russ). From Ref. Zh., Farmakol., Khimioter. Sredstva, Toksikol. 1969, Abstr. No. 5.54.674. For methylethylpyridine-HCl (I) and dimethylpyridine-HCl (II) given orally to rats, the LD₅₀ was 1460 and 200 mg/kg, resp.; for mice the values were 1684 and 1560 mg/kg. S.c. values for rats were 555 and 567, and for mice 441 and 453 mg/kg; i.p. values were 435 and 408 for rats, and 384 and 453 mg/kg for mice. The effects of these drugs resembled those of narcotics. I and II are synergists of urethane, antagonists of barbital; they forestall convulsions induced by cocaine, picrotoxin, and augment the effect of nicotine and arecoline on N- and M-choline receptors of the central nervous system. I is a synergist to harmine, while II is an antagonist. The rate of rendering II harmless in vivo is less than that for I, while II has a greater capability for accumulation. **MORW***

2126b Toxicology of aromatic hydrocarbons. Uzdavani, E. R.; Lisnyanskii, E. Z.; Karimulina, N. K.; Pshippova, Z. Kh.; Talalaev, V. M. (USSR). *Toksikol. Gig. Prod. Neftekhim. Neftekhim. Proizvod. 1968, 126-7 (Russ). From Ref. Zh., Khim. 1969, Abstr. No. 111443. Toxic properties of some C₁₀-C₁₄ derivs.: dodecylbenzene (I), pseudocumene (1,2,4-trimethylbenzene) (II), durenene (1,2,4,5-tetramethylbenzene) (III), dipseudocumylmethane (IV), and 2-isopropylphthalene (V) were studied. The substances were expressed in the following order of toxic properties (from low toxic to relatively harmless); III, IV > II > V > I. They comprised an order of II > V, I > III, IV by the strength of the local irritating effect. The irritating effect on rabbit eye increased in the order I < V < II. **NBRK***

2127c Carcinogenicity testing of selected food additives by parental administration to infant Swiss mice. Epstein, Samuel S.; Fujii, Keiji; Andrea, J.; Mautel, Nathan (Lab. of Environ. Pathol., Child. Cancer Res. Found., Inc., Bethesda, Md.). *Toxicol. Appl. Pharmacol. 1970, 18(2), 321-34 (Eng). The toxicity and carcinogenicity of 6 food additives, safrole; alginate; polyoxyethylene-(20)-sorbitan monostearate (Tween 60); 6-ethoxy-2,2,4-trimethyl-1,2-dihydroquinoline (Santoquin); 1,3,5-trimethyl-2,4,6-tris-(3,5-di-tert-butyl-4-hydroxybenzyl)benzene (Ionox 390); 2,4-bis(4-hydroxy-3,5-di-tert-butylphenoxy)-6-(m-oxylthio)-1,3,5-triazine (RA-858) were tested by 4 consecutive i.p. injections in mice, aged 1, 7, 14, and 21 days. Doses of safrole, alginate, Tween 60, or Santoquin in excess of 1 mg on day 1 of life were acutely toxic; Ionox and RA-858 were non-toxic at doses of 10 mg. Surviving mice were sacrificed at 1 yr. After a total dosage of 6.6 mg safrole, a low incidence of multiple pulmonary adenomas, 6%, and pulmonary adenocarcinomas, 10%, and a high incidence of hepatomas 58%, developed in 31 male mice alive at weaning; in contrast with a zero incidence of multiple pulmonary adenomas and pulmonary adenocarcinomas, and a 5-6% incidence of hepatomas in uninjected and solvent-injected controls, based, resp., on 36 and 78 males alive at weaning. In groups tested with alginate and RA-858, tumor incidences fell within control ranges; carcinogenicity data for Santoquin and Ionox were equivocal. These results confirm the practical utility of neonates for carcinogenicity testing in that remote tumors develop rapidly following restricted parental administration of relatively small quantities of test materials. **RCZB***

2128d Influence of pharmacologic or physiologic pretreatment on acute daunomycin cardiac toxicity in the hamster. Herman, Eugene H.; Schein, Philip S.; Farmer, R. M. (Microbiol. Assoc., Inc., Bethesda, Md.). *Toxicol. Appl. Pharmacol. 1970, 16(2), 335-44 (Eng). Daunomycin (NSC 82151), an antibiotic effective in the treatment of acute leukemia, has produced a lethal cardiopulmonary syndrome in humans and a specific type of acute bidirectional arrhythmia in the hamster. An arrhythmic dose of daunomycin (50 mg/kg) produced a mild pressor response and an increased concn. of plasma epinephrine and norepinephrine. The arrhythmia can be prevented by either destroying the central nervous system or by pretreatment with reserpine. Both mecamylamine and guanethidine significantly increased the arrhythmic dose, but hexamethonium caused only minor effects. The protective effect of hexamethonium might have been limited by a short duration of action in the hamster. Phenoxybenzamine failed to prevent the arrhythmias while propranolol either did not change or increased the arrhythmic dose only slightly. Propranolol has been shown to depress the myocardium, and daunomycin may also exert similar activity. The possibility exists that the cardiodepressant properties of the 2*



TECHNICAL DATA

DI-CUP® PEROXIDE

BULLETIN ORC-204C
(Supersedes ORC-204B)

DI-CUP® DICUMYL PEROXIDE AND ITS DECOMPOSITION PRODUCTS SUMMARY OF TOXICOLOGICAL INVESTIGATIONS

When used as a peroxidic catalyst, Di-Cup® dicumyl peroxide is always present in conjunction with its decomposition products (acetophenone, dimethylbenzyl alcohol, and *alpha*-methylstyrene). This bulletin, therefore, has been prepared to summarize the toxicological information obtained on all four compounds. These data are presented in detail on the following pages and are also summarized in Table I, page 6.

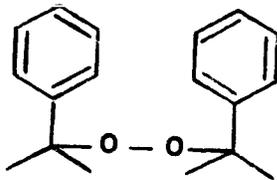
Summary

Di-Cup and its decomposition products are only slightly toxic by ingestion or inhalation. Mild eye and skin irritation may be encountered from accidental exposure to liquids or vapors.

The decomposition products of Di-Cup, however, are strong odorants. Low vapor concentrations result in persistent aromatic scents; when present in high concentrations, these odors may be objectionable.

Chemical Composition

Di-Cup is commercial dicumyl peroxide, available in three forms. The molecular weight of dicumyl peroxide is 270.36; its structural formula is shown below.



General Properties

The four forms of Di-Cup permit selection of material most convenient for the application. Di-Cup 40C and 40KE are white, free-flowing powders that average 40% active material supported on precipitated calcium carbonate and Burgess KE clay, respectively. Di-Cup T, with 90-93% dicumyl peroxide, is a pale yellow, low-melting, semicrystalline solid. Di-Cup R is a pale yellow to white, granular, low-melting crystalline solid, and is a more highly refined form that contains

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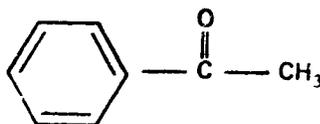
HERCULES INCORPORATED • WILMINGTON, DELAWARE 19898



DECOMPOSITION PRODUCTS

ACETOPHENONE

Acetophenone, also called phenyl methyl ketone and acetylbenzene, is a low-melting solid with a sweet, pungent odor. It is used in perfume bases to impart an orange-blossomlike odor, and in numerous organic syntheses. In the past, it enjoyed limited use as an anesthetic and hypnotic. Its structural formula is shown below.



Physical Properties

Acetophenone has a molecular weight of 120.14, a melting point of 67°F (19.7°C), and a vapor pressure of 1 mm Hg at 99°F (37°C) and 100 mm Hg at 67°F (19.7°C). It is insoluble in water, but soluble in most organic solvents. It has a flash point (closed cup) of 180°F (82°C).

Acute Oral Toxicity

The oral LD₅₀ of acetophenone for rats has been reported as 900 mg/kg, and 3,000 mg/kg, with typical symptoms of anaesthesia and deep coma preceding death.

Acute Dermal Toxicity

The LD₅₀ for guinea pigs by skin absorption of undiluted acetophenone is greater than 20,000 mg/kg.

Eye Irritation

When placed in the eyes of rabbits, undiluted acetophenone caused conjunctival irritation and transient corneal damage comparable in degree to that caused by butyl alcohol.

Skin Irritation

Undiluted acetophenone is a primary skin irritant for rabbits. It has also been reported to cause irritation to human skin in some industrial operations.

Acute Inhalation Toxicity

Because of its low vapor pressure, the inhalation toxicity of acetophenone has been given very little study. Exposure of rats to saturated vapor concentrations (about 600 ppm or 3,000 mg/m³) for 8 hrs produced no deaths.



Acute Oral Toxicity

The oral LD_{50} in the rat was found to be 4,800 mg/kg.

Eye Irritation

Application of two drops in the eyes of rabbits caused slight irritation of the conjunctiva, but no corneal damage.

Skin Irritation

Repeated applications to the skin of rabbits caused moderate to marked erythema. There was no indication of absorption with subsequent systemic toxic effects.

Acute Inhalation Toxicity

Vapor inhalation at 2,920 ppm (14 g/m^3) for 15-60 min caused respiratory irritation and central nervous system depression in rats, mice, and guinea pigs. Mice died after about 4 hrs, but rats and guinea pigs survived the 5-hr exposure.

Inhalation Toxicity

The Threshold Limit Value (TLV⁽¹⁾, 1980) for α -methylstyrene is 100 ppm or 480 mg/m^3 (ceiling). Reduction to 50 ppm (240 mg/m^3) was proposed by the American Conference of Governmental Industrial Hygienists (ACGIH) in 1979. This value probably will become effective in 1981. Available toxicological information is reviewed in the above publication.

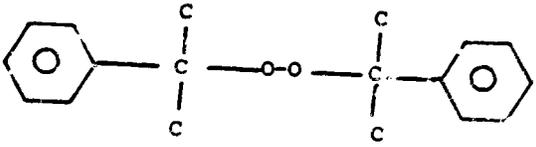
METHANE

Methane is considered a simple asphyxiant by the ACGIH. It has no physiological action except when it lowers the partial pressure of oxygen in the air enough to cause effects due to oxygen deprivation. It has no warning odor. Because of its low toxicity, no TLV has been set.

⁽¹⁾ Registered trademark of American Conference of Governmental Industrial Hygienists.

EFFECTS INFORMATION PROFILE

AUG 19 1983

ID No.	CHEMICAL NAME	SYNONYMS	CAS No.
39	Bis (1-methyl-1-phenylethyl) peroxide	Cumene peroxide dicumylperoxide	80-43-3
Description Solid; strong oxidizing material; may ignite organics on contact		Use Intermediate for acetone, phenol; used as polymerization catalyst, vulcanizing agent.	
Melting point: Vapor pressure (B.P.): Negligible Specific gravity: Water solubility: Organic solubility: log P oct/water: 3.12 Empirical formula: C ₁₈ H ₂₂ O ₂		Structural Formula 	
Biochemical Information		Observations in Humans	
<u>Reference</u>	<u>Nature of Info.</u>	<u>Page</u>	<u>Reference</u>
			<u>Nature of Info.</u>
			<u>Page</u>
			4
			Peterson, et al., (1983)
			Clinical
			5
			Sato, et al., (1980)
			Waste water
			5
			Moham et al., (1982)
			Hazard evaluation
			2
			CAF
			Clement (1978)
			6-10

CURRENT AWARENESS FILE

PEROXIDE, BIS(alpha,alpha-DIMETHYLBENZYL)

000080433

7968

C18-H22-O2

270.40

1X1EBCOX1E1E

ACTIVE DICUMYL PEROXIDE

BIS(alpha,alpha-DIMETHYLBENZYL)PEROXIDE

CUMENE PEROXIDE

CUMYL PEROXIDE

DICUMYL PEROXIDE

DICUMYL PEROXIDE (DOT)

DI-alpha-CUMYL PEROXIDE

DI-CUP

DIISOPROPYLBENZENE PEROXIDE

ISOPROPYLBENZENE PEROXIDE

oxl-rat LD50:4100 mg/kg

DOT-ORGANIC PEROXIDE, LABEL:ORGANIC PEROXIDE

REPORTED IN EPA TSCA INVENTORY, 1980

ON-LINE-TOXICOLOGY DATA BANK-NLM, DECEMBER 1982

NIOSH 13478 estimated people exposed, ACT 9%, TR 36%, GEN 54%, No. OCCS 30

EPA TSCA 8(a) PRELIMINARY ASSESSMENT INFORMATION PROPOSED RULE

salmonella microsomal

BSPIM 1/75-19B

FEREAC 41,57018,76

FEREAC 45,13646,80

SELECTED

0 0 8 4

TOXICOLOGICAL INFORMATION

- MAY
8
 SI - CA/093/143701H
 AU - Yamaguchi T ; Yamashita Y
 AD - Dep. Food Nutr., Yamaguchi Women's Univ., Yamaguchi
 TI - Mutagenicity of hydroperoxides of fatty acids and some hydrocarbons
 SO - Agric. Biol. Chem.; VOL 44, ISS 7, 1980,1675-8
 LA - ENG
 CD - ABCHA
 AB - CSAC COPYRIGHT: CHEM ABS The hydroperoxides of Me linoleate and Me linolenate were mutagenic to Salmonella typhimurium in the Ames mutagenicity test. Of the various types of hydrocarbon peroxides, only hydroperoxide type R-OOH showed mutagenicity, i.e., t-Bu hydroperoxide and cumene hydroperoxide, whereas dialkyl and diacyl peroxides showed no activity. (75-91-2 Tert-Butyl hydroperoxide)(80-15-9 Cumene hydroperoxide) M202 showed no mutagenicity.
 RN - 75-91-2; 80-15-9; 79-21-0; 80-43-3; 94-36-0; 105-74-8; 110-05-4; 937-14-4; 7722-84-1; 11068-03-4; 75036-23-6
 EM - 8011
- MAY
2
 SI - EMIC/60/010642
 AU - CHEVALLIER M ; LUZZATI D
 TI - THE SPECIFIC MUTAGENIC ACTION OF THREE ORGANIC PEROXIDES ON REVERSE MUTATIONS AT TWO LOCI IN E.COLI 15T-9-13
 SO - C R HEBD SEANCES ACAD SCI SER D; 250:1572-1574,1960
 LA - FRE
 CD - CHDDA
 AB - EMIC/ORNL
 KM - SUCCINIC PEROXIDE ; CUMENE PEROXIDE ; THYMINE PEROXIDE ; BACTERIA
 KN - ESCHERICHIA COLI ; JOURNAL
 RN - 123-23-9; 80-43-3
 EM - 0203

OBSERVATIONS IN HUMANS

- SI - TOXBIB/83/174699
AU - Petruson B ; J'arvholm B
AB - Department of Otolaryngology, Sahlgren's Hospital, G'oteborg, Sweden.
TI - Formation of new blood vessels in the nose after exposure to dicumylperoxide at a chemical plant.
SO - Acta Otolaryngol (Stockh); VOL 95, ISS 3-4, 1983, P133-9
LA - Eng
CO - ADLAA
IS - 0001-6489
AB - Eighteen workers exposed to dicumylperoxide in a chemical plant were subjected to examination of the nose by rhinoscopy, mucociliary function test and rhinomanometry. Eight other workers at the plant and 20 hospital workers were used as controls. The mucociliary function and nasal air flow were the same in subjects exposed and those not exposed to peroxide. Nine of the workers exposed to dicumylperoxide had visible blood vessels in the mucosa on the anterior part of the nasal septum. Only 2 persons in the other groups had visible blood vessels. Both had a common cold at the time of the examination. The possibility that dicumylperoxide may initiate formation of new blood vessels is discussed. To test this hypothesis, experiments on laboratory animals will be done with airborne dust containing peroxides.
KW - TOXBIB ; Adult ; Chemical Industry ; Cilia PHYSIOLOGY ; Human
KW - Middle Age ; Mucus PHYSIOLOGY ; Nasal Mucosa #BLOOD SUPPLY
KW - Neovascularization # ; Nose Diseases #CHEMICALLY INDUCED/DIAGNOSIS
KW - Occupational Diseases #CHEMICALLY INDUCED/DIAGNOSIS
KW - Peroxides #ADVERSE EFFECTS ; Respiratory Airflow
RN - 80-43-3
EM - 8306

ENVIRONMENTAL INFORMATION

6 SI - CA/093/137478C
 AU - Sato H ; Nakaya M ; Nouchida M
 TI - Oil adsorbent for wastewater
 SO - Jpn. Kokai Tokkyo Koho PATENT NO. 80 22312 02/18/80 (Mitsubishi Rayon Co., Ltd.)
 LA - JPN
 AB - CBAC COPYRIGHT: CHEM ABS MgO, Mg(OH)₂, or BaSO₄ (as oil-adsorbent filler) 5-60, crosslinkable ethylene-vinyl acetate copolymer 40-95 parts and an org. peroxide 0.2-5% relative to the copolymer are melted at 100-220.degree., pelletized, water cooled, and deaerated to contain .10-0.50% H₂O. (24937-78-8 Ethylene-vinyl acetate copolymer) The product is effective for emulsified oil. Thus, MgO 50, the copolymer (25%) 100, and dicumyl peroxide 0.6 parts were blended for 30 min, extruded to 50 mm diam., pelletized to 3-60 mesh, water cooled, and centrifuged to contain 15% H₂O. (80-43-3 Dicumyl peroxide) When wastewater contg. turbine oil 100 ppm, as a suspension, was passed at linear velocity 8 m/h through the 1 m column to a 10% breakthrough or pressure loss of 1 kg/cm², the oil absorption was 0.76 g/g.
 RN - 24937-78-8; 80-43-3; 1309-48-4

4 SI - CA/096/222539D
 CC - CA/159005
 AU - Mohan VK ; Becker KR ; May JE
 AD - IDL Chem. Ltd., Hyderabad
 TI - Hazard evaluation of organic peroxides
 SO - J. Hazard. Mater.; VOL 5, ISS 3, 1982,197-220
 PT - JOURNAL ARTICLE
 CY - India
 LA - ENG
 CD - JHMAD
 AB - CBAC COPYRIGHT: CHEM ABS Safety org peroxide Org peroxide hazard evaluation Detonability org peroxide Thermal stability org peroxide Explosion hazard org peroxide Fire hazard org peroxide;Combustion Of org. peroxides, potential for Deflagration;Detonation Of org. peroxides, potential for;Explosion Hazards, of org. peroxides, evaluation of;Fire Hazards, of org. peroxides, evaluation of;Peroxides Hazards of, evaluation of Org.
 RN - 80-43-3; 94-36-0; 105-64-6; 614-45-9; 1338-23-4; 77-2-84-1
 EM - 8207

HYDROPEROXIDES AND PEROXIDES

1. tert-Butyl hydroperoxide
2. 2,5-Dimethyl-2,5-bis(tert-butylperoxy)hexane
3. para-Menthane hydroperoxide
4. Cumene hydroperoxide
5. Dicumyl peroxide
6. 1,3-Bis(tert-butyl-dioxyisopropyl)benzene

Working Draft

Prepared by

Clement Associates, Inc.

September 14, 1978

DICUMYL PEROXIDE

I. CHEMICAL AND PHYSICAL INFORMATION

A. Identification

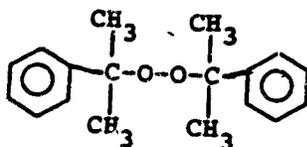
1. CAS No.: 80-43-3
2. NIOSH No.: SD81500
3. Synonyms and Trade Names

Bis(1-methyl-1-phenylethyl)peroxide; peroxide, bis(alpha, alpha-dimethylbenzyl)alpha-cumyl peroxide; active dicumyl peroxide; bis(alpha, alpha-dimethylbenzyl)peroxide; bis(2-phenyl-2-propyl) peroxide; cumene peroxide; cumyl peroxide; di-alpha-cumyl peroxide; Di-Cup; Di-Cup 40C; dicumene hydroperoxide; dicumenyl peroxide; Dicap 40KE; isopropylbenzene peroxide; Luperox 500R; Luperox 500T; Percumyl D; Percumyl D 40; Perkadox B; Perkadox EC; Perkadox SB

(NIH/EPA 1978)

B. Formulas and Molecular Weight

1. Structural Formula



(NIH/EPA 1978)

2. Empirical Formula



(HCP 1976)

3. Molecular Weight

270.4

(NIOSH 1977)

C. Physical Properties

1. Description

Solid

(MITRE 1976)

2. Boiling Point

No information was found in the sources searched.

3. Melting Point

No information was found in the sources searched.

4. Vapor Pressure

Negligible

(MITRE 1976)

5. Solubility

No information was found in the sources searched.

6. Octanol/Water Partition Coefficient

No information was found in the sources searched.

7. Specific Gravity

No information was found in the sources searched.

D. Composition of the Commercial Product

No information was found in the sources searched.

DICUMYL PEROXIDE

II. Source and Fate in the Environment

A. Sources

1. Production and Trends

>1,000 lb (1977) (SRI estimate) (USEPA 1977)

2. Manufacturers and Suppliers

Hercules
Pennwalt Corp. (OPD 1977)

3. Use

As a polymerization catalyst and vulcanizing agent
(COS 1977)

4. Occupational Exposure

Rank: 2,513
Estimated number of persons exposed: 13,000*
*rough estimate (NOHS 1976)

5. Release

No information was found in the sources searched.

B. Environmental Fate

1. Occurrence

No information was found in the sources searched.

2. Transformation

No specific information was found in the sources searched.

EPA comments on physical and chemical data

3. Bioaccumulation

No information was found in the sources searched.

Enclosures

III. Biological Information

A. Effects on Humans

No information was found in the sources searched.

B. Tests on Laboratory Organisms

1. Metabolism

No information was found in the sources searched.

2. Toxic Effects

a. General Toxicity

NIOSH RTECS

Decrease in hemoglobin level, erythrocyte count, total blood protein, blood SH groups, and blood peroxidase activity in rats given cumene peroxide in food for 4 months

b. Carcinogenicity

No information was found in the sources searched.

c. Mutagenicity and Cell Transformation

Induced mutations in tryptophan deficient E. coli 15T⁻9-13.

d. Teratogenicity, Embryotoxicity, and Fetotoxicity

No information was found in the sources searched.

IV. Environmental Effects

A. Ecological Effects

No information was found in the sources searched.

B. Other Environmental Effects

No information was found in the sources searched.

V. Work in Progress

No information was found in the sources searched.

Enclosures

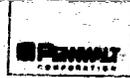
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39

40

41

0 0 9 2



**Di-t-butyl Peroxide
(CAS: 110-05-4)**

Product Literature

Enclosed please find toxicity data, reports of health effects testing, and copies of our technical bulletins and Material Safety Data Sheets.

Annual Production Data and Trends

Confidential Business Information (CBI).
See enclosed envelope marked "TSCA-CBI".

Contains No CBI

Production Worker Exposure

Confidential Business Information (CBI).
See enclosed envelope marked "TSCA-CBI".

Product Use Exposure

Di-t-butyl peroxide is transported primarily in 15- and 55-gallon steel drums. These containers are closed for transport and, therefore, exposure would only result from accidental release of the compound. In use these products are transferred either mechanically or manually. In spite of the relatively high vapor pressure, the low toxicity of this material leads us to believe that no significant risk to the worker using this material is presented. These compounds are consumed in the reaction processes in which they are used and, therefore, release from these processes is limited only to accidental releases.

Environmental Exposure

Di-t-butyl peroxide is produced in an open system. Vaporization losses can be expected throughout the system. However, local exhaust ventilation is anticipated to gather essentially all vaporized material at the individual production sites. The exhaust ventilation is directed to a ventilation scrubber which removes the organic vapors from the air stream. Liquid effluent losses are transported by a pipeline to the plant biological wastewater treatment facility. The effluent of this facility is subjected to deep-well injection. It is anticipated that process losses to the environment are extremely small.

RECEIVED
OPPT/CBI
JUL 14 AM 9:16

11085

Di-t-butyl Peroxide
(CAS: 110-05-4)
Page 2



Toxicological Data

The acute oral LD₅₀, > 25g/kg (rat) and acute inhalation LC₅₀, > 4103 ppm (4 hrs., rat) data as shown on the attached MSDS suggest a very low order of acute toxicity.

11094

OPTIONAL FORM NO. 104 (REV. 9-88)

MATERIAL SAFETY DATA SHEET

"ESSENTIALLY SIMILAR" TO OSHA FORM 20
FORM 4000 (REV. 9-88)

ADDRESS: Penwalt Corporation
Lucidol Division
1740 Military Road
Buffalo, NY 14240

Penwalt Product Name
Di-t-Butyl Peroxide Penwalt Code No. **063**

Chemical Name and Molecular Formula
Di-t-Butyl Peroxide $C_8H_{18}O_2$

Emergency Phone Number(s)
Business: **(716)877-1740**
Other:

Synonyms
Bis (1, 1-dimethylethyl) Peroxide

CAS No.(s) **110-05-4**
Chemical Family
Dialkyl Peroxide

MATERIALS OR COMPONENTS	% w/w
Di-t-Butyl Peroxide	98.5

HAZARD DATA (TLV, LD50, LC50, etc.)

DOT Shipping Name - **Organic Peroxide, Liquid NOS**
Freight Classification - **Chemicals NOIBN**
Hazardous Classification - **Flammable Liquid**
IMCO page - **#5148**

Boiling Point/Range 111.1°C 232°F	Melting Point °C °F	Freezing Point > -40 °C -40 °F	Molecular Weight (Calculated) 146
Specific Gravity (H ₂ O=1) .785 @	Vapor Pressure (mm Hg) °C °F	Vapor Density (Air=1)	
Solubility in H ₂ O insoluble	% Volatiles by Volume	Evaporation Rate <input type="checkbox"/> Ether = 1 <input type="checkbox"/> Water = 1 <input type="checkbox"/> Butylacetate = 1	
Appearance and Odor Colorless, pale, yellow liquid	Other		
Flash Point °C <76 °F	Test Method Seta	Flammable Limits Lower % Upper %	Autoignition Temperature/Fire Point °C °F

EXTINGUISHING MEDIA
 Water-spray water-fog Water stream CO₂ Dry chemical Alcohol foam Foam Earth or sand

SPECIAL FIRE FIGHTING PROCEDURES
 Do not enter building Allow fire to burn Water may cause frothing Do not use water **See ***

UNUSUAL FIRE AND EXPLOSION HAZARDS
 Dust explosion hazard Sensitive to shock Contamination Temperature Other (specify): **See ****

STABILITY
 Stable Unstable

CONDITIONS CONTRIBUTING TO INSTABILITY
 Thermal decomposition Photo degradation Polymerization Contamination

INCOMPATIBILITY - Avoid contact with
 Strong acids Strong alkalis Strong oxidizers Other (specify):

HAZARDOUS DECOMPOSITION PRODUCTS - THERMAL AND OTHER (list)
Decomposition products are flammable.

CONDITIONS TO AVOID
 Heat Open flames Sparks Ignition sources Other (specify):

STEPS TO BE TAKEN IF MATERIAL IS RELEASED OR SPILLED
 Flush with water Absorb with sand or inert material Neutralize Sweep or scoop up and remove Keep upwind. Evacuate enclosed spaces. Prevent spread or spill
vermiculite **non-sparking tools**

WASTE DISPOSAL METHOD - Consult federal, state, or local authorities for proper disposal procedures.

***If larger amount involved, evacuate area and fight fire from safe distance.**
****Heat or contamination may lead to rapid decomposition with gassing.**

CONTINUED ON REVERSE SIDE

NA - Not Applicable.

0095

Before using product, read and follow directions and precautions on product label and bulletin.

Oral (acute)	LD ₅₀ > 25,000 mg/kg (rate)
Dermal (acute)	
Eye	Inhalation (acute) LC ₅₀ > 4103 ppm (4 hrs) rats
Chronic, Subchronic, etc.	
Skin and eye irritation (rabbits) - non-irritating prolonged inhalation of vapors may have inebriatory effect similar to effects of alcohol.	

PERMISSIBLE EXPOSURE LIMIT (Specify if TLV/TWA or Ceiling (c))		Other:	
ACGIH 19	OSHA 19		
IRRITATION	<input type="checkbox"/> Skin <input type="checkbox"/> Eye	<input type="checkbox"/> Severe <input type="checkbox"/> Moderate	<input type="checkbox"/> Moderate <input type="checkbox"/> Mild (transient)
CORROSIVITY	<input type="checkbox"/> Skin <input type="checkbox"/> Eye	<input type="checkbox"/> 4 hrs. (DOT) <input type="checkbox"/> May cause blindness	<input type="checkbox"/> 24 hrs. (CPSC)
SENSITIZATION	<input type="checkbox"/> Skin <input type="checkbox"/> Respiratory	<input type="checkbox"/> Allergen	INHALATION EFFECTS <input type="checkbox"/> Narcotic effect <input type="checkbox"/> Cyanosis <input type="checkbox"/> Asphyxiant
LUNG EFFECTS (Specify):			
OTHER (Specify): <input type="checkbox"/> Repeated contact - skin defatter <input type="checkbox"/> Other (Specify):			
INGESTION	<input type="checkbox"/> Induce vomiting <input checked="" type="checkbox"/> Do NOT induce vomiting	<input type="checkbox"/> Give plenty of water	<input type="checkbox"/> Get medical attention <input type="checkbox"/> Other (specify):
DERMAL	<input checked="" type="checkbox"/> Flush with soap and water <input type="checkbox"/> Get medical attention	<input type="checkbox"/> Contaminated clothing - remove & launder	<input type="checkbox"/> Contaminated shoes - destroy <input type="checkbox"/> Other (specify):
EYE CONTACT	<input checked="" type="checkbox"/> Flush with plenty of water for at least 15 minutes	<input checked="" type="checkbox"/> Get medical attention	<input type="checkbox"/> Other (specify):
INHALATION	<input checked="" type="checkbox"/> Remove to fresh air <input checked="" type="checkbox"/> If not breathing, give artificial respiration	<input type="checkbox"/> Give oxygen	<input type="checkbox"/> Get medical attention <input type="checkbox"/> Other (specify):

VENTILATION REQUIREMENTS - Always maintain exposure below permissible exposure limits			
<input type="checkbox"/> Consult an industrial hygienist or environmental health specialist	<input checked="" type="checkbox"/> Local exhaust	<input checked="" type="checkbox"/> Use with adequate ventilation	<input type="checkbox"/> Check for air contaminant and oxygen deficiency
Other (specify):			
EYE	<input type="checkbox"/> Face shield <input checked="" type="checkbox"/> Safety glasses <input type="checkbox"/> Goggles	HAND (GLOVE TYPE) <input type="checkbox"/> Polyvinyl chloride <input checked="" type="checkbox"/> Neoprene	<input type="checkbox"/> Butyl rubber <input type="checkbox"/> Natural rubber <input type="checkbox"/> Polyvinyl alcohol <input type="checkbox"/> Poly-ethylene <input type="checkbox"/> Other (specify):
RESPIRATOR TYPE - Use only NIOSH / MESA approved equipment			
<input type="checkbox"/> Self-contained	<input type="checkbox"/> Supplied air	<input checked="" type="checkbox"/> Can or cartridge gas or vapor	<input type="checkbox"/> Filter - dust, fume, mist <input type="checkbox"/> Other (specify):
OTHER PROTECTIVE EQUIPMENT			
<input type="checkbox"/> Rubber boots	<input type="checkbox"/> Apron	<input type="checkbox"/> Other (specify):	

PRECAUTIONARY LABELING			
<input type="checkbox"/> Wash thoroughly after handling	<input type="checkbox"/> Do not get in eyes, on skin or clothing	<input type="checkbox"/> Do not breathe dust, vapor, mist, gas	<input type="checkbox"/> Keep container closed
<input checked="" type="checkbox"/> Do not store near combustibles	<input type="checkbox"/> Keep from contact with clothing and other combustible materials	<input type="checkbox"/> Empty container may contain hazardous residues	<input type="checkbox"/> Use explosion proof equipment
<input checked="" type="checkbox"/> Keep away from heat, sparks, and open flames	<input checked="" type="checkbox"/> Store in tightly closed containers	<input type="checkbox"/> Other (specify):	
Other handling and storage conditions			
Flammable liquid under DOT regulations (red label)			

Prepared by	Date	Address	Phone
Dennis C. Cardino	11/10/80	1740 Military Rd., Buffalo, NY	716/877-1740

PLEASE NOTE: The above information is accurate to the best of our knowledge. However, since data, safety standards, and government regulations are subject to change and the conditions of handling and use, or misuse are beyond our control, Pennwalt MAKES NO WARRANTY, EITHER EXPRESS OR IMPLIED, WITH RESPECT TO THE COMPLETENESS OR CONTINUING ACCURACY OF THE INFORMATION CONTAINED HEREIN AND DISCLAIMS ALL LIABILITY FOR RELIANCE THEREON. User should satisfy himself that he has all current data relevant to his particular use.

Di-(1-hydroperoxycyclohexyl) Peroxide
CAS# 2699-12-9

Test	Result	References
Acute Oral Toxicity (mice)		
60% in DBP	LD ₅₀ 900 mg/kg LD ₅₀ 850 mg/kg	CA 73 23807z 1970 "
Primary Skin Irritation (rabbits)	Irritating	"
Primary Eye Irritation (rabbits)	Irritating	"

1-Hydroperoxy-1'-hydroxy-dicyclohexyl Peroxide
CAS# 78-18-2

Test	Result	References
Acute Oral Toxicity (mice)		
60% in DBP	LD ₅₀ 880 mg/kg LD ₅₀ 740 mg/kg	CA 73 23807z 1970 "
Primary Skin Irritation (rabbits)	Irritating	"
Primary Eye Irritation (rabbits)	Irritating	"

DIALKYL PEROXIDES

Di-t-butyl Peroxide
CAS# 110-05-4

Test	Result	References
Acute Oral Toxicity (rats)		
Acute Oral Toxicity (mice)	LD ₅₀ >25,000 mg/kg	F&S
Acute Intraperitoneal Toxicity (rats)	LD ₅₀ >4000 mg/kg LD ₅₀ >50 ml/kg	W&T KNC-71
Acute Inhalation Toxicity (rats)	LD ₅₀ 3210 mg/kg LD ₅₀ 4572 mg/kg	F&S CA 74 12377: 1971
Acute Inhalation Toxicity (rats)	LD ₅₀ > 4103 ppm (4 hrs.)	F&S
Skin Irritation (rabbits)	Non-irritating	F&S

KEY TO REFERENCES

- ACGIH** American Conference of Governmental Industrial Hygienists. TLV Listing - 1981 Edition.
- ACC** Arco Chemical Company -- Internal Reports.
- BJM** British J. Ind. Medicine 27, 11-12 (January 1970)
- B.P. 826** British Patent 1,040,826 - 9/1/66.
- CA** Chemical Abstracts.
- CIVO** Central Instituut voor Voedingsonderzoek TNO (CIVO), Zeist, Holland -- Reports for Akzo Chemie.
- | | | | | | |
|--------|-----------|---------|-----------|--------|----------|
| R-4707 | June 1975 | R-5340 | Aug 1977 | R-5601 | Jan 1978 |
| R-9-76 | Sept 1976 | R-9-77 | Sept 1977 | R-5619 | Jan 1978 |
| R-5150 | Oct 1976 | R-5519 | Oct 1977 | R-5624 | Feb 1978 |
| R-5170 | Nov 1976 | R-11-77 | Nov 1977 | R-6-79 | Jun 1979 |
| R-5171 | Nov 1976 | R-5568 | Dec 1977 | R-6141 | Aug 1979 |
| R-5341 | May 1977 | R-5574 | Dec 1977 | R-6143 | Aug 1979 |
| | | R-5599 | Jan 1978 | R-6304 | Dec 1979 |
| | | | | R-6366 | Feb 1980 |
- F & S** Floyd, E.P., and Stokinger, H.E., Am. Ind. Hygiene Assoc. J. 19, No. 3, 205 (1958).
- FDRL-50** Food & Drug Research Laboratories inc. N.Y.C. [Reports to R.T. Vanderbilt Co. Ind. dated Sept. 18 and Nov. 25, 1959.]
- FDRL** Food & Drug Research Laboratories Inc., Waverly, N.Y. [Report to Lucidol Division, Pennwalt Corporation.]
- FMC** Data supplied by letter dated April 17, 1972 from H.M. Castrantas. FMC Corporation to Organic Peroxide Producers Safety Division of P.I.
- HJK** H.J. Kühle - Zbl. Arbeits Med. 8, 25 (1958)
- H-ORC-204C** Hercules Bulletin ORC-204C
- H-ORC-304B** Hercules Bulletin ORC-304B
- H-OP-524A** Hercules Bulletin OP-524A
- HEW-76** U.S. Department of Health, Education and Welfare. National Institute for Occupational Safety and Health "Registry of Toxic Effects of Chemical Substances - 1976 Edition".
- HYSAAV** Hygiene and Sanitation 29, 103 (January 1964) (English Translation of Gigena Sanitariya).
- IBT** Industrial Bio Test Laboratories, Inc. of Northbrook, Ill. Reports to PPG Industries, Inc.
- | | | | |
|-----------|---------|-----------|---------|
| IBT-A341 | 9/16/71 | IBT-A8766 | 7/27/70 |
| IBT-A8559 | 7/15/70 | IBT-A8767 | 8/24/70 |
- IBT-H** Industrial Bio-Test Laboratories, Inc., Northbrook, Illinois. Reports to Hercules Incorporated.
- | | | | |
|--------|-------------------|--------|--------------------|
| 76-13A | December 20, 1976 | 76-13D | September 28, 1978 |
| 76-13B | November 3, 1976 | 77-21 | |
| 76-13C | December 15, 1976 | | |
- IHFA** Industrial Hygiene Foundation of America, Inc. Pittsburgh, Pa. Reported dated May-June 1961 to PPG Industries, for "The Acute Oral Toxicity of Pure isopropyl Percarbonate".

KEY TO REFERENCES (Cont.)

IRDC

International Research and Development Corporation, Mattawan, Michigan.

(a) Reports to LUCIDOL DIVISION, Pennwalt Corporation.

IRDC #1	5/27/63	IRDC 164-017	7/17&70
IRDC 164-006	6/30/64	IRDC 164-021	6/4/72
IRDC 164-007	12/22/64	IRDC 164-073	2/8 & 8/14/78
IRDC 164-008	1/29/65	IRDC 164-076	7/28/78
IRDC 164-010	11/19/64	IRDC 164-089	2/ 5/80
IRDC 164-011	8/26/66	IRDC 164-090	2/ 7/80
IRDC 164-012	8/26/66	IRDC 164-091	2/15/80
IRDC 164-013	4/30/67	IRDC 164-092	2/15/80
		IRDC 164-093	2/15/80
		IRDC 164-094	3/ 3/80
		IRDC 164-095	2/14/80

(b) Reports to Organic Peroxide producers Safety Division, The Society of the Plastics Industry, Inc.

IRDC 328-001	8/31/73	IRDC 328-006	2/27/74
IRDC 328-002	8/31/73	IRDC 328-007	8/23/76
IRDC 328-003		IRDC 328-008	8/23/76
IRDC 328-004		IRDC 328-009	8/23/76
IRDC 328-005			

(c) Reports to Aztec Chemicals - Division of Dart Industries, Inc.

IRDC 376-007	7/28/77	IRDC 376-010	12/15/78
IRDC 376-008	7/6 & 10/2/78	IRDC 376-011	5/17/79
IRDC 376-009	7/24 & 9/11/78		

(d) Reports to Noury Chemical Corporation.

IRDC 378-001	7/15/76	IRDC 378-008	7/24/73
IRDC 378-002	7/15/76	IRDC 378-011	8/ 9/78
IRDC 378-004	12/19/76	IRDC 378-013	1/25/80
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EYE SAFETY

BULLETIN 20.17

In the interest of furthering the safe use of organic peroxides, Lucidol has published papers and safety information. With our desire to keep the users of peroxides well informed, we have translated and abstracted the following article on eye safety from PLASTICA, published in Delft, Holland.

HYGIENIC NOTES CONCERNING CATALYSTS USED IN THE MANUFACTURE OF PLASTICS

Organic peroxides are used as catalysts in a wide number of polymerization reactions. The liquid peroxides are quite often used as they are received or like the solid or paste catalysts they are made into solutions in various solvents before adding to a reaction. Handling of these solutions may result in industrial accidents. The splashing of peroxide solutions into the eyes of plant or laboratory personnel should be guarded against.

Kuchle (1958) and Floyd (1958) investigated the effect on the eyes of rabbits and their results are summarized below:

The Effect of Organic Peroxides on Rabbit Eyes

<u>Peroxide</u>	<u>Form and Concentration at Application</u>	<u>Effect L M S</u>	<u>Remarks</u>
• Lauroyl Peroxide	Powder	X	After 1 minute eye flushed with water
• Benzoyl Peroxide	Powder 93%	X	"
	Paste 50%	X	"
• Di-t-Butyl Peroxide	Liquid	X	
• t-Butyl Hydroperoxide	75% Solution	X	
	35% in propylene glycol	X	
	7% in propylene glycol	X	
• t-Butyl Perbenzoate	50% in dimethyl phthalate	X	
• t-Butyl Peracetate	50% in dimethyl phthalate	X	After 1 minute eye flushed with water
Cyclohexanone Peroxide	50% solution in cyclohexanone	X	" (effect increases upon
	50% paste in dimethyl phthalate	X	(aging or
	40% liquid	X	charge
• Diacetyl Peroxide	30% solution in dimethyl phthalate	X	

<u>Peroxide</u>	<u>Form and Concentration at Application</u>	<u>Effect L M S</u>	<u>Remarks</u>
Methyl Ethyl Ketone Peroxide	4% in dimethyl phthalate	X	
	3% in dimethyl phthalate	X	
	0.6% in dimethyl phthalate	X	

Code: L - indicates very slight temporary damage
M - moderately serious damage that can be treated successfully
S - a strong or very strong effect with lasting residual defects which would include cloudiness of the cornea or even total destruction.

Tests were also conducted by these authors to determine the effect of flushing the eyes with water. The importance of having eye flushing fountains available and flushing the eyes as soon as possible is pointed out by the following:

1. Flushing the eyes within four seconds showed a preventative effect.
2. Flushing the eyes after 30 seconds had some beneficial effect.
3. Flushing the eyes after 60 seconds had no effect.

Flushing the eyes with a 2% sodium bicarbonate solution showed some beneficial effects. Coating the eye with oil (Vitamin A containing Vogan oil*) tended to increase the harmful effects of the peroxide solutions in many cases.

Little is known about the poisoning effect of peroxides and no reports of damage to respiratory channels have been received. In 1958 Floyd listed the following peroxides in order of decreasing toxic effect as follows:

Methyl ethyl ketone peroxide is more toxic than cumene hydroperoxide or t-Butyl Hydroperoxide and these are more toxic than Di-t-Butyl Peroxide.

The tests were carried out on rats, mice and rabbits and Di-t-Butyl Peroxide actually shows little or no toxic effect. Horgan (1957) also shows that t-Butyl Hydroperoxide was more toxic than Di-t-Butyl Peroxide when tested on rats.

On the basis of the above, the following recommendations are made:

1. Safety glasses should be worn.
2. The best first aid consists of a generous, prolonged stream of water that is continued for at least 10 minutes.
3. Flushing should be carried out immediately (on the spot of the accident).
4. Flushing with water as outlined in 2 and 3 above is preferred over treatment with small quantities of antidotes.
5. Oils or ointments should not be used.

The data contained herein are based on the above mentioned publication and are believed to be correct. They are presented here without comment. No opinion or warranty is expressed or implied regarding the accuracy of these data.

*Merck - Germany

Toxicity #5

Reprinted from *ANALYTICAL CHEMISTRY* Vol. 28, No. 2, June, 1956
Printed in U.S.A.

Toxicity Studies of Certain Organic Peroxides and Hydroperoxides*

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U. S. Department of Health, Education, and Welfare, Cincinnati, Ohio

ORGANIC peroxides are likely constituents of certain types of oxidizing smog^{2,3,4,5} and important as industrial catalysts, intermediates, and raw materials for synthesis.⁶ Many of them are abundant sources of free radicals. For these reasons tests have been conducted in our laboratory to determine the toxicity of these compounds on small mammals. Specific compounds were selected on the basis of their known use in industry, as type constituents of oxidizing smog, their availability, and the feasibility of their use for extensive tests.

Materials and Methods

PHYSICAL AND CHEMICAL PROPERTIES OF PEROXIDES

Some of the characteristics of the organic peroxides used, viz. di-*t*-butyl peroxide, *t*-butyl hydroperoxide, cumene hydroperoxide, and methyl ethyl ketone peroxide, are given in Table I; their specifications are given in Table II. Most of these values were furnished by the manufacturers.

The compounds were used as received from the manufacturer except when dilution was necessary, in which event propylene glycol, or in the case of methyl ethyl ketone peroxide, dimethyl phthalate was used.

POLAROGRAPHIC METHOD OF MEASUREMENT

Because the conventional chemical methods (iodide or stannous chloride) are not specific for organic peroxides, whereas the polarographic method distinguishes between peroxides and hydroperoxides and is specific for determining both,⁷ this method was selected as the most desirable for this study in which mixtures of compounds were involved.

Polarographic measurements were made with a Sargent Model XXI Visible-Recording Polarograph, using a dropping mercury electrode assembly and an improvised saturated calomel

electrode which made contact with the test solution by way of an agar-KCl bridge. This agar bridge was suspended over the test solution (1:1 benzene:methanol) during the de-aeration period, then lowered into the solution before recording the polarogram. The polarographic method was that of Willits, et al.,⁸ although the electrolysis vessel was of one author's (E.P.F.) design, patterned somewhat after that of Bruscheiler and Minkoff.⁹ According to Willits, et al.,⁸ both the hydroperoxide and peroxide half-wave potentials are widely separated and the polarographic method not only identifies the functional groups but also gives a quantitative measure of each in peroxide-hydroperoxide mixtures. Di-*t*-butyl peroxide is an exception to this in that it is not reduced polarographically.

ANIMAL SPECIES AND TECHNIQUES

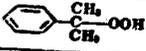
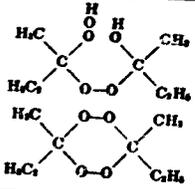
The rats used in these experiments were Wistar-derived adult, male, albinos weighing approximately 200 gm at the beginning of each test. The mice were Swiss-derived adult, male, albinos having an initial average weight of 20 gm each. The rabbits were white males of the New Zealand strain weighing from 2.7-6.5 kg.

Standard laboratory pellets and drinking water were available to all animals at all times except during exposure or fasting periods. The rats were housed five to a cage, the mice, ten to a cage, and the rabbits, one to a cage. The rats and mice were sacrificed by cervical dislocation; the rabbits, by overdosage of Nembutal.

Acute studies were performed by administering organic peroxides by the intraperitoneal and oral routes on rats, and by the inhalation route on both rats and mice. The calculated LD₅₀ values for the intraperitoneal and oral routes were determined according to Weil¹⁰ in which five rats were used for each of four geometrically spaced dosage levels. Three of the organic peroxides were diluted (volume/volume) as follows to accomplish easier intraperitoneal administration: 20% *t*-butyl hydroperoxide in propylene glycol, 10% cumene hydroperoxide in propylene glycol, and 5% methyl ethyl ketone peroxide in dimethyl

* Presented at the 12th Annual Meeting American Industrial Hygiene Association, St. Louis, Mo., April, 1957.
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TABLE I
Properties of Organic Peroxides Used

Compound	Structural Formula	M.W.	Sp.G.	M.P. C°	B.P. C°(mm Hg)	E _{1/2} Volts
Di-t-Butyl Peroxide	(CH ₃) ₂ COOC(CH ₃) ₂	146.22	0.794 20/4	-40		
t-Butyl Hydroperoxide	(CH ₃) ₂ COOH	96.12	0.805 20/4	-3 to -19	111 (700) 80 (204)	-1.00
Cumene Hydroperoxide		152.18	1.046 15.6/ 15.6		65 (.18)	-0.93
Methyl Ethyl Ketone Peroxide ^a		ca. 105.	1.12 15/15		d. 118	-1.00

^a Polarographic half-wave potentials were corrected for IR drop, but were determined on the compounds as received from the manufacturer without further purification. Table II indicates the purity of these compounds. Willits, et al.⁸ report the E_{1/2} of pure t-butyl hydroperoxide and cumene hydroperoxide as -0.96 and -0.68 volt respectively.

phthalate. In all other cases the peroxides were used as received from the manufacturer without further dilution. The rats used for oral tests were fasted 24 hours previous to treatment. Six rats and ten mice were used for each exposure level for the inhalation studies. These exposure levels were determined by measuring the liquid volume of the compound used for the duration of the exposure (15 liters of air/minute for four hours) and computing the concentration. Polarographic analysis of occasional samples

(10 liters per minute for 5 minutes each) of the chamber atmosphere for organic peroxide gave concentration values ranging from 91% to 102% of these calculated values, with an average of 97%. Air from the laboratory compressed-air line was cleaned and dried before passing into the exposure chamber. Some of this air was passed through an aerosol unit (containing the liquid organic peroxide) at a measured rate of flow. This inhalation-exposure apparatus was constructed of glass and patterned after one used by Svirbely and Saltzman.¹²

Subchronic tests, to study the possible cumulative effects and the resultant histopathology were performed on rats by repeated intraperitoneal and oral doses one-fifth that of the LD₅₀ three times weekly (Monday, Wednesday, Friday) for seven weeks.

A histopathologic study involving serial sacrifices was made on rats injected intraperitoneally in an attempt to find some consistent pathologic change due to an organic peroxide. The rats were given sublethal doses of organic peroxides in three injections during one week (Monday, Wednesday, Friday) and one-third of the group sacrificed at 1, 2 and 3 weeks after the first injection. An unexposed control group of rats of the same age was sacrificed with the exposed group.

For testing the toxicity of organic peroxides on the rabbit eye, the technique of Draize and Kelly¹³ was used, by which the reactions observed in the cornea, iris, and the palpebral and

TABLE II
Specifications of Organic Peroxides Used

Compound	Manufacturer ^a	Per Cent Purity (Minimum)	Per Cent Active Oxygen (Minimum)	Other Components
Di-t-Butyl Peroxide	Lucidol	97	10.6	Fe (trace)
t-Butyl Hydroperoxide	Lucidol	70	12.5	Di-t-B.P. (20%)
Cumene Hydroperoxide	Hercules	73	7.7	H ₂ O (0.4%), Parent Hydrocarbons, and derivatives
Methyl Ethyl Ketone Peroxide	Cadet & Lucidol	60	11.0	Dimethyl phthalate (40%)

^a Lucidol: Division of Wallace & Tiernan, Inc., 1740 Military Road, Buffalo 5, New York; Hercules: Hercules Powder Co., Wilmington 99, Delaware; Cadet: Cadet Chemical Corporation, Burt, New York.

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bulbar conjunctivae were scored separately. This method of assigning numerical scores gives as much as 80% of the weight to the observed lesions in the cornea and iris, the structures of the eye most concerned with vision. The ocular reactions were read with the aid of a hand slit-lamp.

Skin tests for primary irritation were performed on a similar group of rabbits by the standard technique used in this laboratory by which a large area of the back of each rabbit was sheared closely, and one or two drops of each compound applied at a different spot on this sheared area (as many as six spots per rabbit), and spread to a circular area about two centimeters in diameter. At each reading the rabbit was sheared and the area wiped clean with a wet cloth for subsequent readings which were made at 24, 48 and 72 hours respectively. The severity of the reaction was graded as follows: 0 for negative, 1 for erythema, 2 for erythema and edema, 3 for erythema, edema and slight vesiculation, 4 for erythema, edema and severe vesiculation or bullous formation.

To test for possible changes in serum protein, rabbits were treated as in the above tests for primary irritation, using one rabbit per compound. Electrophoretic patterns were made on the serum from 3-5 ml of blood taken from the rabbit's ear before and after exposure. The Spinco Paper Electrophoresis Cell, Model R-Series D, with the Spinco Duostat Regulated D. C. Power Supply, and the Spinco Analytrol Recording Scanner and Integrator for translating the dye densities into "ticks" were used to test for changes in serum protein. The technique was that of Durrum.¹⁴

Tests for methemoglobin according to the technique of Evelyn and Malloy¹⁵ were made on blood secured from the rat heart by the method of Burhoe.¹⁶ The Beckman Ratio-Recording Spectrophotometer Model DK-2 was used to record the per cent light transmission from 350 to 700 $m\mu$ wave length.

Results of Acute Tests

INTRAPERITONEAL INJECTIONS, RATS

Methyl ethyl ketone peroxide, t-butyl hydroperoxide and cumene hydroperoxide were more toxic by all routes examined by a factor of from 40-150-fold than di-t-butyl peroxide as shown by the LD₅₀ values given in Table III. All of the rats showed signs of weakness and some loss of equilibrium following single doses of all but the lowest levels of each of the above four organic peroxides. Prostration occurred frequently at the higher dose levels and was usually followed

by death, although some of the rats recovered completely. This was particularly conspicuous in the animals treated with methyl ethyl ketone peroxide in which there was one survivor of five rats treated with 80 mg/kg and five survivors of five treated with 40 mg/kg. Prostration had occurred in all. Porphyrin deposition in the nostrils occurred in many of the rats following a single injection of cumene hydroperoxide (200 mg/kg) and di-t-butyl peroxide (2000 to 5000 mg/kg). The pelage was coarse in most of the rats at two to five days following a single dose (excepting the lowest) of each of the four organic peroxides. Shivering occurred in rats following high doses of di-t-butyl peroxide. Practically all of the deaths from intraperitoneal injection of organic peroxides in these acute studies occurred within six days. There was no weight loss in any of the surviving animals during the four-week period following a single injection at each dose level, however.

ORAL ADMINISTRATION, RATS

The LD₅₀ value for di-t-butyl peroxide by gavage was greater than 25,000 mg/kg; amounts greater than this distended the rat's stomach beyond the point where the results would have toxicologic significance.

The three hydroperoxides were found to have LD₅₀ values of the same order of magnitude ranging from 382 mg/kg for cumene hydroperoxide to 484 mg/kg for methyl ethyl ketone peroxide (Table III).

Practically all of the deaths from the oral administration of organic peroxides occurred within five days. There was no weight loss in any of the surviving rats during the four-week period following a single dose administration of each dose level. Extensive urinary bleeding occurred in the rats treated with cumene hydroperoxide (400 mg/kg).

INHALATION EXPOSURE, RATS AND MICE.

The LC₅₀ values (Table III) were comparable for rats and mice, the greatest divergence again occurring in the case of di-t-butyl peroxide; 4103 ppm, was the highest attainable vapor concentration under the conditions of the experiment and neither rats nor mice succumbed from a 4-hour exposure at this level. Tertiary-butyl hydroperoxide by inhalation tests is seen to be less toxic also than either methyl ethyl ketone peroxide or cumene hydroperoxide, whereas they were found to be of approximately equal toxicity by the intraperitoneal route (65 and 95 mg/kg) or by oral administration (484 and 382 mg/kg).

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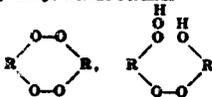
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TABLE III
Toxicity Limits of Four Organic Peroxides

Compound	LD ₅₀		LC ₅₀		Maximal Non-Irritating Strength	
	mg Compound/kg Body Weight		ppm 4 hours exposure		Per Cent Peroxide in Vehicle	
	Intra-peritoneal	Oral (Gavage)	Inhalation		Skin	Eye
	Rats	Rats	Rats	Mice	Rabbits	Rabbits
Di-t-Butyl Peroxide (ROOR)	3210	>20000	>4103	>4100	57	57
t-Butyl Hydroperoxide (ROOH)	57	608	800	300	35	7
Cumene Hydroperoxide (ROOH)	65	353	330	300	7	1
Methyl Ethyl Ketone Peroxide	65	684	300	170	1.5	0.6



Rats exposed to di-t-butyl peroxide vapor (4103 ppm) developed head and neck tremors uniformly in all six rats after ten minutes of exposure. A weakness in the extremities occurred, appearing first in the forelegs, later in the hindlegs. After 45 minutes the tremors lessened in all the rats. After 1 hour and 45 minutes one of the rats showed signs of hyperactivity at 10-second intervals. At the end of the 4-hour exposure the tremors had virtually disappeared, and the rats remained prostrate. Seven days later the hyperactive rat died; the only death of the six exposed rats.

The mice were less affected than the rats, exhibiting only excitability and somewhat labored breathing. This occurred after ten minutes of exposure, was maximal at 30 to 50 minutes, and still persisted, though somewhat lessened, at the end of the exposure period. The high dosage levels of each of the peroxides tested by the inhalation route caused porphyrin deposition in the nostrils and irregular respiration in the majority of the rats and mice.

SKIN TESTS, RABBITS

There was apparently no immediate discomfort caused by the direct cutaneous application of the organic peroxides; the delayed reaction was quite severe, however, for three of the compounds, t-butyl hydroperoxide, methyl ethyl ketone peroxide, and cumene hydroperoxide. When applied full strength these three compounds caused erythema, edema and vesiculation within two or three days. Methyl ethyl ketone peroxide again exhibited the greatest toxicity of the four organic peroxides tested, di-t-butyl

peroxide the least. The maximal nonirritating strengths of the peroxides tested are given in Table III.

EYE TESTS, RABBITS

The maximal nonirritating strengths of these peroxides are given in Table III. The total scores expressing the effects of various concentrations of organic peroxides on the eye mucosa are given in Table IV. With the exception of di-t-butyl peroxide, strong solutions of organic peroxides in dimethyl phthalate or propylene glycol when applied directly to the eyes of rabbits affected the cornea, iris, and conjunctiva extensively. Weaker solutions (Table IV) affected

TABLE IV
Toxicity of Organic Peroxides to Rabbit Eye Mucosa*

Compound	Strength %	Day of Reading Following Treatment						
		1	2	3	4	5	7	
Di-t-Butyl Peroxide	97	0	0	0	0	0	0	
t-Butyl Hydroperoxide	35†	59	57	72	75	0	46	
t-Butyl Hydroperoxide	7†	4	13	8	0	0	0	
Cumene Hydroperoxide	10‡	59	59	77	75	0	44	
Cumene Hydroperoxide	1‡	11	6	4	0	0	0	
Methyl Ethyl Ketone Peroxide	3‡	87	52	11	9	0	7	
Methyl Ethyl Ketone Peroxide	0.62	0	4	0	0	0	0	
Control	0	0	0	0	0	0	0	

* Ocular lesion score of Drazin & Kelly.²

† Dilutions made with propylene glycol.

‡ Dilutions made with dimethyl phthalate.

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only the conjunctiva causing redness of the palpebral conjunctiva and chemosis. Methyl ethyl ketone peroxide, which is a mixture of dimeric peroxide and hydroperoxide, was found to be particularly marked as an eye irritant. Washing the rabbits' eyes with water four seconds after application of the peroxides prevented reactions in every case.

Results of Repeated Administration

INTRAPERITONEAL INJECTIONS, RATS

With dosages of 1/4 the intraperitoneal LD₅₀ thrice-weekly for 7 weeks, cumene hydroperoxide and t-butyl hydroperoxide, each produced death in one of five rats; methyl ethyl ketone peroxide killed two of five; whereas di-t-butyl peroxide killed none during the 7-week period, as shown in Table V. All of the rats gained weight normally throughout the test period, although the pelage of some was noticeably coarse.

ORAL ADMINISTRATION, RATS

Table V shows that methyl ethyl ketone peroxide produced death in five of five rats treated under the same dosage schedule described for repeated intraperitoneal injections, cumene hydroperoxide killed four of five, di-t-butyl peroxide, two of five, and t-butyl hydroperoxide, none during the 7-week test period. Loss of weight, or the failure to gain normally, was a conspicuous feature of this test. The pelage was coarse in most of the rats after the first week of treatment.

Pathology

ACUTE TESTS

Autopsy of several of the mice and rats killed by the exposure to organic peroxide vapor or sacrificed within the first 24 hours following exposure showed hyperemia of the lungs, with petechial hemorrhages on the lung surface of some and gross hemorrhage in others. No other lesion found in the acute studies (by inhalation, oral, and intraperitoneal routes) by either gross or histologic examination could be attributed to organic peroxides. However, there was occasional damage to the liver (fatty changes in liver cells in central portion of lobules, increase in number of round cells in portal spaces, or mild hyperemia), and to the kidney (granular precipitate or casts in the lumina of the convoluted or collecting tubules, and desquamation of the epithelium of the proximal tubules).

TABLE V
Mortality of Rats from Repeated Doses of Organic Peroxides
Five Animals Used per Test.
Dosage: 1/4 LD₅₀ of each route, three times weekly on alternate days.

Organic Peroxide	Cumulative Mortality by Weeks													
	Intraperitoneal							Oral (Gavage)						
	1	2	3	4	5	6	7	1	2	3	4	5	6	7
Di-t-Butyl Peroxide	0	0	0	0	0	0	0	1	2	2	2	2	2	2
t-Butyl Hydroperoxide	0	0	1	1	1	1	1	0	0	0	0	0	0	0
Cumene Hydroperoxide	0	1	1	1	1	1	1	4	4	4	4	4	4	4
Methyl Ethyl Ketone Peroxide	1	1	1	1	1	2	2	1	2	2	2	4	4	4

SERIAL SACRIFICE STUDY

In the rats injected with t-butyl hydroperoxide there was some depletion of glycogen in the liver and the liver cells were slightly more homogeneous than in the controls, but no structural changes were observed. A number of rats had chronic interstitial pneumonia, apparently unrelated to the exposure.

In the rats injected with methyl ethyl ketone peroxide the liver was mildly damaged in all. All rats at first week sacrifice showed depletion of liver glycogen and dissociation of liver cords. At two and three weeks there was still low glycogen content but no dissociation of liver cells. The control rats showed none of these changes, but these changes are frequently found in the liver due to agonal stress. Chronic interstitial pneumonia and bronchiectasis were seen in a large percentage of rats and were consistent with the findings in spontaneous murine pneumonia.

Results of the Special Tests

CROSS-TOLERANCE

Experiments were performed to determine whether cumene hydroperoxide would afford protection from subsequent lethal concentrations of itself, hydrogen peroxide, ozone and nitrogen dioxide separately. For this, a group of 45 mice was exposed to an atmosphere of 100 ppm cumene hydroperoxide for six hours. (The LC₅₀ by inhalation is 220 ppm for a 4-hour exposure). The mice in groups of ten were challenged one week later to the vapors of either cumene hydroperoxide, hydrogen peroxide, ozone and nitrogen dioxide at the 4-hour lethal concentration or above it. As a control, a group of ten mice of the same age and weight not pre-

TABLE VI
Comparison of Albumin/Globulin Ratios in the
Serum of Rabbits Treated Cutaneously
with Organic Peroxides

	Day of Reading Following First Application							
	0*	1	2*	5*	7	9	12	14
Di-t-Butyl Peroxide	1.0	1.4	1.2	1.7	1.8	2.0	1.4	2.0
t-Butyl Hydroperoxide	1.0	1.0	1.1	1.1	1.2	1.2	1.2	1.4
Cumene Hydroperoxide	1.3	1.5	1.3	1.0	1.2	1.2	1.5	1.4
Methyl Ethyl Ketone Peroxide	1.2	1.2	1.3	1.1	1.1	1.5	1.4	1.6
Propylene Glycol	1.3	1.7	1.2	1.7	1.3	1.4	1.2	2.0
Dimethyl Phthalate	1.4	1.5	1.6	1.4	1.3	1.8	1.8	1.6

* 0.1 ml of compound applied to a different area of the rabbit's back (after clipping) on each of these dates.

viously exposed to cumene hydroperoxide accompanied the pre-exposed mice when challenged by each of the four substances. Cumene hydroperoxide afforded protection only against hydrogen peroxide vapors. Challenging concentrations of hydrogen peroxide at 226 ppm for four hours (the approximate LC_{50} for mice) resulted in a mortality of 10% of the pre-treated mice, against 50% mortality for the controls. No protection was afforded against the other respiratory irritants, including cumene hydroperoxide.

METHEMOGLOBIN FORMATION IN RATS

It was found that methyl ethyl ketone peroxide formed methemoglobin in rat blood *in vitro*, but not *in vivo*. Repeated daily exposures of rats by inhalation at low levels for three days in succession, or repeated intraperitoneal injections three times a week for five weeks failed to develop any significant amount of methemoglobin.

CHANGES IN SERUM PROTEINS.

The albumin/globulin ratio increased appreciably over a 2-week period (three applications and eight readings as indicated in Table VI) for rabbits treated as in the tests for primary irritation with di-t-butyl peroxide, t-butyl hydroperoxide and methyl ethyl ketone peroxide. But it also increased similarly in rabbits treated with propylene glycol and dimethyl phthalate, and not at all for rabbits treated with cumene hydroperoxide.

Discussion

The toxicity values in Table III are expressed as pure compounds, although as seen in Table II, none was absolutely pure and three of them

contained appreciable amounts of stabilizing vehicles. The toxicity limits of the four organic peroxides determined in these studies revealed marked differences. Particularly noteworthy was the finding that the hydroperoxide (ROOH) was far more toxic than its dimeric peroxide (ROOR), by all routes of administration. Toxicity studies reported elsewhere support this finding; dicumyl peroxide was found to have an oral LD_{50} (single dose for rats) of 3500-4000 mg/kg compared with 382 mg/kg for cumene hydroperoxide found by the present authors. This same report⁷ indicated that dicumyl peroxide was relatively nonirritating to rabbit eyes, whereas the present authors found cumene hydroperoxide to be extremely irritating to rabbit eyes. Although the methyl ethyl ketone substance was considered a peroxide, it was actually a mixture of peroxide and hydroperoxide, as noted earlier; its toxicity bears this out. As a group, one would rate the organic peroxides, according to the classification of Hodge and Sterner⁸ as "moderately toxic" (oral LD_{50} , single dose, rats) although one of them, di-t-butyl peroxide, would be classed as "relatively harmless". By the inhalation route the classification would be moderately toxic⁹ and "slightly toxic" respectively.

One possible correlation, between the degree of toxicity and the properties of these compounds (Tables I and II) may be found in the polarographic half-wave potential, $E_{1/2}$. Di-t-butyl peroxide, the least toxic of the group, was not reduced by the polarographic technique, whereas the other organic peroxides, t-butyl hydroperoxide, methyl ethyl ketone peroxide, and cumene hydroperoxide, which as a group are "moderately toxic" compounds, have comparable half-wave potentials (-0.92 to -1.09 volts).

The physiologic responses in the acute tests were mild except for the head and neck tremors described for rats and mice exposed to di-t-butyl peroxide vapor. The most common response was that of weakness and coarse pelage, which was particularly conspicuous following intraperitoneal injections. Nasal porphyrin exudate occurred occasionally in the acute intraperitoneal and inhalation tests. Most of the rat deaths in the acute studies occurred within 48 hours after the administration of organic peroxides, and practically all of the deaths occurred within 5 or 6 days. Oddly, gain in weight was normal in all of the acute tests, as well as during the 7-week injection tests, but not in the 7-week oral tests.

The skin and eye tests indicated that the hydroperoxides, cumene hydroperoxide, t-butyl

hydroperoxide were not immediately irritating to organic peroxide from the reaction.

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Summa

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hydroperoxide, and methyl ethyl ketone peroxide were irritants, although their effects were not immediate; di-t-butyl peroxide was not irritating to either the skin or eyes. None of the organic peroxides caused irritation when washed from the rabbits' eyes four seconds after application.

The fact that animals died from repeated administration of small doses ($\frac{1}{2}$ LD₅₀) of organic peroxides is interpreted as a cumulative effect, and probably of considerable importance because in most instances (Table V) cumulative deaths occurred by intraperitoneal as well as the oral route. No explanations are given to account for why di-t-butyl peroxide did not show cumulative toxicity intraperitoneally when it was rather marked orally; nor why the hydroperoxide showed no cumulative mortality orally. There was no conspicuous physiologic response to the repeated intraperitoneal injections except for the development of rather coarse pelage in some of the rats. The weight gain was normal throughout the test period. The more marked cumulative mortality resulting from the oral administrations would indicate lesser detoxication by this route. Associated with this was a conspicuous loss of weight and development of coarse pelage in all of these tests.

There was no pathologic change that could be attributed specifically to the organic peroxides. Changes in the liver were typical of those frequently found following agonal stress, and the lung changes were considered consistent with those found in spontaneous murine pneumonia. The lungs of some rats and mice were found by gross examination to be hyperemic and slightly hemorrhagic following exposure to organic vapors.

Of the special tests performed with the organic peroxides it was found that rats following exposure to the vapor of cumene hydroperoxide developed an appreciable tolerance to the challenging lethal doses of the vapors of hydrogen peroxide, although oddly no tolerance to cumene hydroperoxide itself could be demonstrated. Another test showed that whereas methyl ethyl ketone peroxide produced methemoglobin in rat blood *in vitro*, repeated inhalation exposures and intraperitoneal injections of methyl ethyl ketone peroxide failed to produce methemoglobin in rat blood *in vivo*.

Summary

Of the four organic peroxides studied (methyl ethyl ketone peroxide, cumene hydroperoxide, t-butyl hydroperoxide, and di-t-butyl peroxide),

methyl ethyl ketone peroxide was the most toxic by all five routes of administration. Toxicity ratings indicate that the hydroperoxides (ROOH) are "moderately toxic" compounds. Di-t-butyl peroxide (ROOR) was the least toxic by all routes tested and is classed as "relatively harmless" to "slightly toxic" (inhalation).

Histopathologic study failed to reveal any site of damage, although there were questionable indications that the liver may be involved.

Some protection from lethal doses of hydrogen peroxide was demonstrated in rats following exposure to cumene hydroperoxide and subsequent challenging with hydrogen peroxide vapors.

It was demonstrated in rats for at least three of the four organic peroxides tested that repeated sublethal doses ($\frac{1}{2}$ LD₅₀) either orally or intraperitoneally resulted in cumulative effects ending in death of some of the animals.

All of the organic peroxides tested were skin and eye irritants, except di-t-butyl peroxide.

Changes in the electrophoretic pattern of the serum protein of rabbits, or the presence of methemoglobin in rat blood could not be conclusively demonstrated in animals following exposure to organic peroxides.

Acknowledgments

We wish to acknowledge the following persons for assisting in this study: Dr. Richard Mendenhall for the electrophoresis work, Dr. Olga Dobrogorski for the histopathology study, Dr. J. L. Svirbely for the "cross-tolerance" experiment involving hydrogen peroxide, Vernon B. Perone for the rabbit skin and eye tests, and Dr. Jacob Berghuis for the eye mucosa readings.

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enhanced by the addn. of activated charcoal to the dialysis soln. RCZB

123266b Human placental hydroxylation of 3,4-benzopyrene during early gestation and at term. Juchau, Mont R. (Sch. Med., Univ. Washington, Seattle, Wash.). *Toxicol. Appl. Pharmacol.* 1971, 18(3), 665-75 (Eng). Benzopyrene hydroxylase activity in human placental tissues was investigated during early gestation (8-16 weeks) to det. if cigaret smoking would produce increased hydroxylation capacity at this gestational stage. Particulate subfractions of term placental homogenates from women who smoked cigarets during pregnancy exhibited relatively high levels of enzymic activity. At 8-10 weeks gestation, however, levels of enzymic activity in homogenates of human placenta or fetal livers were undetectable regardless of maternal smoking habits. At 11-13 weeks gestation, very low levels of hydroxylase activity were obsd. in placentas of smokers and slightly higher levels were apparent in smoker placentas at 14-16 weeks gestation. Hydroxylating capacity of placental homogenates from nonsmokers was not detected at 8-16 weeks gestation. Steroids synthesized by human placental tissues, i.e., β -estradiol, estrone, and progesterone, markedly inhibited the placental-catalyzed hydroxylation of benzopyrene. Cholesterol, dehydroepiandrosterone, testosterone, and androstenedione, which serve as substrates for other placental mixed-function oxidase systems, however, exhibited comparatively minor inhibitory effects. Similar effects of these and other steroids (methyltestosterone and pregnenolone) were obsd. on the placental hydroxylation of 3-methylcholanthrene pretreated rats. RCZB

123267c Alterations of bromsulphthalein metabolism in chronic alcoholism. Rainer, H.; Schneck, H. (I. Med. Universitätsklinik, Wien, Vienna, Aust.). *Wien. Klin. Wochenschr.* 1971, 83(10), 168-9 (Ger). Bromsulphthalein (I) excretion studies were made in 2 groups with very high and moderate alc. consumption. In correspondence with histol. findings, these patients showed marked changes in I metabolism with decreased maximal excretion, plasma disappearance, half-life, and increased I retention. Paper-chromatographic studies showed that these findings are due to decreased I conjugation. V. N. Nekrassoff

123268d Effect of a short period of fluoride ingestion on dental fluorosis in cattle. Suttie, John W.; Faltin, E. C. (Coll. Agric. Life Sci., Univ. Wisconsin, Madison, Wis.). *Amer. J. Vet. Res.* 1971, 32(2), 217-22 (Eng). Ingestion of 2.5 mg F/kg by 2 groups of heifers, one during the 13th to 15th months of age and the other during the 16th to 18th months, caused severe dental fluorosis esp. in the second group. F anal. of consecutive chronol. sections of avascular enamel indicated that there was a regular pattern of enamel apposition from the top to the bottom of the crown of one incisor before the top of the crown of the next incisor calcified. Data collected showed that a measurement of F content provided an accurate estn. of the period and duration of the exposure of the animal to F. David B. Sabine

123269e Physical dependence on and tolerance to alcohol in the rat. Cicero, Theodore J.; Snider, S. R.; Perez, V. J.; Swanson, L. W. (Sch. Med., Washington Univ., St. Louis, Mo.). *Physiol. Behav.* 1971, 6(2), 191-8 (Eng). Withdrawal of EtOH (7%, 154 days) from rats resulted in extremely hyperactive animals which appeared to be engaged in frantic, highly disorganized, exploratory behavior in an open field, in marked contrast to control rats receiving water. Alcoholic rats were also less responsive to an injected EtOH dose than control rats, even though there was no difference in the rate of disappearance of EtOH from the blood. This suggested the development of a cellular alc. tolerance after a chronic exposure period. EtOH intake, which appeared to exceed the rats' ability to metabolize it, increased progressively throughout the initial exposure and remained unchanged when water was simultaneously offered. BQJN

123270y Change in the acid-alkali equilibrium in rabbits during the administration of only hexachlorobutadiene or hexachlorobutadiene with vitamin E in a subacute test. Popovich, M. I. (Kishinev. Med. Inst., Kishinev, USSR). *Zdravokhranenie* 1970, 13(2), 20-2 (Russ). Hexachlorobutadiene (I) 10 mg/kg was administered to 10 rabbits for 20 days and 10 mg/kg of I plus vitamin E (150 mg/kg) was administered to 12 rabbits for 20 days. A progressive lowering of wt. was obsd. in all animals. The mean loss of wt. by the end of the intoxication period was 494 g in the 1st group and 145 g in the 2nd group. Results of the anal. of blood (pH and other indexes) and urine (pH, titr. acidity, and other indexes) are summarized. It was concluded that the administration of vitamin E leads to normalization of the acid-alkali equil. and its use was recommended. J. Pich

123271z Toxicology of new stabilizers and vulcanizing agents. Belova, G. B.; Shurupova, E. A.; Stankevich, V. V. (USSR). *Sov. Issled. Eff. Khim. Polim. Mater.* 1969, No. 3, 466-75 (Russ). From *Ref. Zh., Biol. Khim.* 1970, Abstr. No. 9F2034. The LD₅₀ values are: Ca dibenzoate 2.3 and 4.0 g/kg, N,N'-di-nitroso-N,N'-diethylamine (?) 1.88 and 0.6 g/kg, N,N'-di-

thio-thiomorpholine 3.4 and 6.7 g/kg for a single administration to mice and rats. Product C-1 and polyphenol No. 9 did not have acute and subacute toxicity. Ca dibenzoate did not cumulate and was only slightly toxic at a daily single dose of 10% of the LD₅₀ value. Dimethylamine and dithiomorpholine derivs. had cumulative properties and had neg. effect on Hb of the blood, general condition, body wt., and wt. of internal organs and irritated the skin and mucosa. NBRL

123272a Effect of gravity on positional alcohol nystagmus (PAN). Oosterveld, W. J. (Univ. Amsterdam, Amsterdam, Neth.). *Aerosp. Med.* 1970, 41(5), 557-60 (Eng). Humans were given 50 ml of pure alc. in a period of 30 sec., the rabbits an unspecified amt. Weightlessness was evoked by a parabolic flight in an airplane lasting up to 12 sec. Positional alc. nystagmus was abolished by weightlessness for several min. L. N. Ellis

123273b Effect of nitrogen mustard intoxication on glucose absorption from the small intestine of the rat. Leibowitz, Michael J.; Merker, P. C. (Coll. Pharm. Sci., Columbia Univ., New York, N.Y.). *Gut* 1971, 12(2), 123-5 (Eng). Nitrogen



mustard (I) (6 mg/kg) given i.p. to rats did not significantly reduce glucose absorption from the small intestine when absorption was adjusted for water movement and dry intestinal wt. and length. When absorption was adjusted only for water movement, it was significantly reduced by I. Thus, alterations in the absorption of glucose by the whole rat are attributable to losses of tissue mass. Intestinal tissue remaining after acute I treatment apparently retains the ability to transport glucose to essentially the same extent as normal intestinal tissue. B.K.J.N.

123274c Effects of carbon monoxide exposure on th arterial walls. Astrup, Poul; Kjeldsen, Knud; Wanstrup, John (Dep. Clin. Chem., Rigshosp., Copenhagen, Den.). *Ass. N.Y. Acad. Sci.* 1970, 174(Art. 1), 294-300 (Eng). Lipoproteins, like many other macromols., pass into the vascular walls, from which they are transported back to the blood through the vasa vasorum or the lymph system. The greater the permeability, the greater the transport. An increased permeability of the vessel walls can explain the enhancing effect of hypoxia and CO exposure on the development of atherosclerosis. Moderate CO exposure (20% carboxyhemoglobin) leads to a considerable increase in the vascular permeability for albumin in normal human individuals. The enhancing effect of CO exposure on atherosclerotic development is due to an increase in the vascular permeability for macromols. In smokers with intermittent CO exposure, little or no increase occurs in the Hb concn. Harry W. Gordon

123275d Histological and histochemical findings in experimental lead enteropathy. Di Nunno, C.; L'Abbate, N.; Strada, L.; Lo Storto, A.; Altamura, B. M. (Ist. Med. Leg., Univ. Bari, Bari, Italy). *Lav. Um.* 1970, 22(8), 360-74 (Ital). Cytochrome oxidase, succinic dehydrogenase, and lactic dehydrogenase activities of both gastric mucosa and intestinal epithelium (duodenum, jejunum, and colon) were studied by means of histol. and histochem. methods. Atrophy of villi, as well as gradual decrease in cytochrome oxidase and succinic dehydrogenase activity were detected. These changes are related to both spasmodic action of Pb and its ability to inactivate SH-groups. Felix Saunders

123276e Hepatic siderosis following estrastilbene dosage in mice. Simon, Hansjoerg; Jaeger, J.; Stoetznner, H.; Kemmer, Chr. (Pathol. Inst., Med. Akad. "Carl Gustav Carus," Dresden, Ger.). *Exp. Pathol.* 1971, 5(1/2), 11-19 (Ger). Fe storage in the mouse liver was studied following s.c. or i.m. administration of estrastilbene D. The estrastilbene-induced siderosis of the hepatocytes was a result of an activated external resorption and a functional change of the hepatocytes. The findings were interpreted as a consequence of increased apoferritin and transferrin production. V. N. Nekrassoff

123277f Toxicology of some organic peroxides-tertiary butyl derivatives. Saotoukii, I. V.; Ivanov, G. V.; Avkhimenko, M. M.; Golubovich, E. Ya.; Karamzina, N. M.; Chirkova, E. M.; Germanova, A. L.; Migukina, N. V.; Mel'nikova, L. V. (USSR). *Toxikol. Gig. Prod. Neftekhim. Neftekhim. Prirod.* 1968, 98-7 (Russ). From *Ref. Zh., Farmakol., Khimioter. Sredstva, Toksikol.* 1969, Abstr. No. 6.54.836. With intragastric administration of *tert*-butylperacetate (I), *tert*-butylperbenzoate (II), and *di-tert*-butylperoxide (III) to mice the LD₅₀ was 632, 914, and 457 mg/kg, resp. A decrease in the rate of the conditioned reflex formation and wave-like excitability changes of the nervous system, displacements as viewed from the hematogenic apparatus, kidney function, decrease in the amt. of normal spermatogonia, and changes in nucleic acid content in the testes were revealed under continuous inhalation of I (exposure, general duration and concn. not indicated). Cumulative properties of II and III were less pronounced than with I. II and III did not have specific effect on the gonads. Min. functional impairments were obsd. under repeated in-

halotico were a III/I. Injections of (I) at 100 mg/kg effects on rabbits. Olla, G. Cagliari, (Ital). Rabbits (0.2 ml of 0.1 LD₅₀) leucine and dehydrogenase changes;

123279h: Behavior intoxicatio G.; Spina (Italy). F activities c wt. 2 kg) s 2 ml dimer (for rabbits) aminopepti all showed i all the enzy hr after the intoxication of the hepat

123280b Behavior of intoxication. S.; Spinazzi (Italy). Foli Rabbits (av region with wt. (approx. 30, and 45 d; concn., factor sively). They vary from nor

123281c E Effects of sm ptoetic tissue G.; Satta, G. Cagliari, (Ital). Rabb region of 0.2 (approx. 0.1 I decreases in I (including neu of the develop showed an incre correspondin erythroblasts. as well as prote.

123282d I, I, Phu-Lich; Cluc Mec. Action B Fr.). C. R. Aca

hepatotoxic solv when administere sts, the resultin into the urine as was also transform 123283e Comp in neonatal and Bernard Abraham *Toxicol. Appl. P* sensitivity of neon than that of adult nervous system, re the blood levels at (LD₅₀) were 2-3 tim.

123284f Blood v dogs. Reves, Pharmacol., Med (C.) *Toxicol. Ap*

... of 0.05 mg II/A. Statistically significant changes were not observed in mice under repeated inhalation of 0.8 mg II/A. The LD50 for the air of dimethylformamide is reported as 0.001 mg/l. for I, 0.001 for II and 0.001 for III.

123276 Experimental dimethylformamide intoxication. Effects of small doses of DMFA on the plasma enzyme picture of rabbits. Zedda, Silvia; Carta, G.; Cascio, G.; Fressa, A.; Olla, G.; Spinazzola, A. (Ist. Med. Lav., Univ. Cagliari, Cagliari, Italy). *Folia Med. (Naples)* 1969, 82(11), 777-86 (Ital). The activities of some plasma enzymes were studied in rabbits (av. wt. 2 kg) s.c. injected daily in the dorsal region with 0.2 ml of dimethylformamide (DMFA)/kg body wt. (approx. 0.1 LD50) for up to 45 days. Glutamic-oxalacetic transaminase, leucine aminopeptidase, sorbitol dehydrogenase, and glutamate dehydrogenase all showed increases, but there was no significant change in the plasma pseudocholinesterase activity. Such changes appear due to parenchymal necrosis caused by DMFA.

123277a Experimental dimethylformamide intoxication. IV. Behavior of some serum enzyme activities in acute DMFA intoxication. Zedda, Silvia; Carta, G.; Cascio, G.; Olla, G.; Spinazzola, A. (Ist. Med. Lav., Univ. Cagliari, Cagliari, Italy). *Folia Med. (Naples)* 1969, 82(11), 768-76 (Ital). The activities of some serum enzymes were studied in rabbits (av. wt. 2 kg) s.c. injected in the dorsal region with a single dose of 0.2 ml of dimethylformamide (DMFA)/kg body wt. (approx. 0.1 LD50 rabbits). Aldolase, glutamic-oxalacetic transaminase, leucine aminopeptidase, alk. phosphatase, and sorbitol dehydrogenase all showed increased activities after 0, 12, and 24 hr. However, the enzymic activities had returned to normal by 48 and 96 hr after the treatment. The changes brought about by DMFA intoxication seemed to be caused by an altered permeability of the hepatic cell.

123277b Experimental dimethylformamide intoxication. III. Behavior of some blood clotting factors in prolonged DMFA intoxication. Zedda, Silvia; Carta, G.; Cudoni, S.; Zinni, S.; Spinazzola, A. (Ist. Med. Lav., Univ. Cagliari, Cagliari, Italy). *Folia Med. (Naples)* 1969, 82(11), 759-67 (Ital). Rabbits (av. wt. 2 kg) were s.c. injected daily in the dorsal region with 0.2 ml of dimethylformamide (DMFA)/kg body wt. (approx. 0.1 LD50) for 45 days. Exams. were made 15, 30, and 45 days from the beginning of the expt. Prothrombin concn., factor VII concn., and factor V concn. decreased progressively. The remaining blood clotting factors did not significantly differ from normal values.

123281c Experimental dimethylformamide intoxication. II. Effects of small repetitive doses of DMFA on hemolymphatic tissue in rabbits. Spinazzola, A.; Zedda, S.; Carta, G.; Satta, G.; Sirigu, M. T. (Ist. Med. Lav., Univ. Cagliari, Cagliari, Italy). *Folia Med. (Naples)* 1969, 82(11), 747-58 (Ital). Rabbits received daily s.c. injections in the dorsal region of 0.2 ml dimethylformamide (DMFA)/kg body wt. (approx. 0.1 LD50) for 45 days. Extended treatment caused changes in Hb values, erythrocyte counts, and leukocytes (including neutrophilic granulocytes and lymphocytes). Anal. developmental stages of the erythroblasts in bone marrow and an increase of basophilic erythroblasts accompanied by corresponding decrease of both polychromatic and oxyphilic thrombocytes. DMFA appeared to inhibit cell reproduction well as protein synthesis.

23282d 1,1,1,2-Tetrachloroethane metabolism. Nguyen-Lich; Chuet, Jean L.; Dutertre-Catella, Helene (UER c. Action Med. Toxiques, Univ. Rene-Descartes, Paris). *C. R. Acad. Sci., Ser. D* 1971, 272(8), 1173-6 (Fr). The



atotoxic solvent, C2Cl4, underwent dehalogenation when administered intragastrically to rabbits, guinea pigs, and the resulting metabolite, C2Cl3OH, being eliminated in the urine as urochloric acid (I). In the rat, C2Cl4 also transformed into C2Cl3OH.

123283e Comparison of the lethality of inhaled diethyl ether neonatal and adult rats. Schwetz, Bernard A.; Becker, and Abraham (Coll. Med., Univ. Iowa, Iowa City, Iowa). *Appl. Pharmacol.* 1971, 18(3), 703-6 (Eng). The toxicity of neonatal rats to inhaled Et2O was 5-6 times less than that of adult rats, possibly due to the immature central nervous system, rather than due to a lower absorption of ether. Blood levels at the respective values of mean time to death were 2-3 times greater in neonatal than in adult rats.

123284f Blood volume following acute ethyl alcohol ingestion logs. Reyes, Joseph G.; Newman, Walter H. (Dep. Pharmacol., Med. Univ. South Carolina, Charleston). *Toxicol. Appl. Pharmacol.* 1971, 18(3), 693-4 (Eng).

The blood vol. fluctuations are inconsequential in acute cardiovascular expts. performed during 6 hr following EtOH ingestion. Hematocrit, blood alc., and plasma vol. were detd. at intervals following treatment of dogs with EtOH (2 g/kg, orally) by a simple method utilizing a single injection of radiolabeled serum albumin.

123285g Development of newborn mice during prolonged treatment with interferon. Greener, Ion; Bourali, Chantal (Lab. Viral Oncol., Inst. Rech. Sci. Cancer, Villejuif, Fr.). *Eur. J. Cancer* 1970, 6(6), 583-6 (Eng). Daily s.c. administration of concd. mouse brain interferon preps. was well tolerated by newborn AKR and C3H mice, and no evidence of toxicity was obsd. as detd. by: overall mortality; the growth curve of treated mice; the wts. of various organs (thymus, spleen, liver, kidney); and by histolog. examn. of the thymus gland. This apparent lack of toxicity of exogenous mouse brain interferon was in contrast to the reported toxicity for lab. animals of various nonviral inducers of endogenous interferon.

123285h Interaction of lipopolysaccharides and lipid A with complement. Galanos, Chris; Rietschel, Ernst; Luederitz, Otto; Weisbach, Otto (Max-Planck-Inst. Immunbiol., Freiburg/Br., Ger.). *Eur. J. Biochem.* 1971, 19(1), 143-52 (Eng). A number of lipopolysaccharides derived from *Salmonella* and *Escherichia coli* S and R mutant strains were tested for toxicity and anticomplementary activity in the absence of added antiserum. Although all preps. were toxic, only a few exhibited high anticomplementary activity, while others proved to be of low or negligible activity. Isolated lipid A from both active and inactive lipopolysaccharides was strongly anticomplementary as well as toxic, when made water-sol. with the aid of suitable carriers. Treatment of R form lipopolysaccharide with Mg++ or Ca++ led to complete pptn. of the lipopolysaccharide with consequent loss of toxicity and anticomplementary activity. This treatment had practically no effect on the anticomplementary activity and toxicity of S form lipopolysaccharides. When lipopolysaccharide, after reaction with complement, was reisolated and purified, the resulting prep. was nontoxic and of negligible anticomplementary activity. No detectable alterations in either the sugar or the fatty acid compn. could be detected. The only significant change was the loss of soly. in water. Treatment of the reisolated lipopolysaccharide with EDTA completely restored soly. in water, toxicity, and anticomplementary activity.

123287j Mycoflora, aflatoxins and free fatty acids in California cottonseed during 1967-1968. Ashworth, L. J., Jr.; McMeans, J. L.; Houston, Byron R.; Whitten, M. B.; Brown, Charles Malcolm (Dep. Plant Pathol., Univ. California, Berkeley, Calif.). *J. Amer. Oil Chem. Soc.* 1971, 48(3), 129-33 (Eng). In central California, neither fungal infections nor aflatoxins are significant problems in cottonseed during the receiving and storage seasons. However, in southern California, the 1967 harvest contained a relatively high percentage of seed invaded before harvest by fungi, including *Aspergillus flavus*. Seed infection and concns. of aflatoxins in seed increased significantly during the time between harvest and storage in southern California. For a short time during storage, seed infection by *A. flavus* increased because of the moisture the seed received late in the season; however, aflatoxin concns. in seed did not increase in storage. The aflatoxin content of the seed removed from storage was a reflection of the relative amt. of aflatoxins the seed contained when they were received for storage. In 1967, the conditions that existed in the large, densely packed seed pile did not favor accumulation of aflatoxins in seed, even though *A. flavus* was active.

123288k Experimental endotoxin shock. Effect of hypothermia on outcome. Williams, Thomas B.; Cavanagh, Denis (Sch. Med., St. Louis Univ., St. Louis, Mo.). *Amer. J. Obstet. Gynecol.* 1970, 108(8), 1171-4 (Eng). An extracorporeal technique of inducing hypothermia is described as it was applied to 3 groups of dogs. All 4 dogs given the hypothermia technique survived. None of the 5 dogs given endotoxin (lipopolysaccharide of *Escherichia coli* in a 5 mg/kg body wt. dose) survived. The blood pressure in the 10 dogs given both endotoxin and hypothermia appeared more nearly normal at the end of 1 hr than in the 2nd group but even then only 1 dog survived for 36 hr. The theoretical advantages of hypothermia were not borne out in practice.

123289m Effects of *Naja nigricollis* venom on blood and tissue histamine. Mohamed, Ahmed H.; El-Serougi, M.; Hamed, R. M. (Fac. Med., Ein-Shams Univ., Cairo, UAR). *Toxicol.* 1971, 9(2), 109-72 (Eng). In dogs, *N. nigricollis* venom produced a marked increase in blood histamine and release of tissue histamine. This latter effect was inhibited by EDTA and Egyptian polyvalent antivenin (contg. no specific antivenin against *N. nigricollis* venom).

123290e Effect of *Naja nigricollis* venom on blood clotting. Mohamed, Ahmed H.; El-Serougi, M.; Hamed, R. M. (Fac. Med., Ein-Shams Univ., Cairo, UAR). *Toxicol.* 1971, 9(2), 173-6 (Eng). *N. nigricollis* venom had an in vivo anticoagulant effect which was heat-labile and was prevented by protamine

TABLE # 2
Oral Toxicities in Mice of some LUPRACO Compounds

(This information was prepared by the Pharmaceutical Laboratory of Wallace & Tiernan, Inc. at Bellville, New Jersey)

Compound Tested	Dose mg/kg.	Mortality	Toxicological Signs	LD ₅₀ mg/kg
LUPRACO C08	4000	0/6	None	4000
LUPRACO C02	4000	0/6	None	4000
	2000	0/6		
	1000	0/6		
2,4-Diethyl Pterostide	4000	1/6	Excitation and slight hyperventilation	4000
	2000	3/6	at the highest dosage levels.	
	1000	0/6		
LUPRACO D01	1000	6/6	Severe depression, cyanosis, and mild tonic convulsions at the highest dosage levels with deaths due to respiratory arrest. Mild intestinal irritation.	470
	750	5/6		
	500	4/6		
LUPRACO #7	2000	4/6	Moderate depression at the highest dosage level only	1900
	1500	0/6		
	1000	0/6		
LUPRACO J08-85	4000	5/6	Depression, cyanosis and mild tonic convulsions. Deaths due to respiratory arrest.	2000
	2000	3/6		
	1000	1/6		
t-Butyl Hydroperoxide	1000	6/6	Severe depression, incoordination, and cyanosis at highest levels. Deaths due to respiratory arrest. Mild intestinal irritation.	710
	750	3/6		
	500	0/6		
t-Butyl Perbenzoate	4000	5/6	Moderate depression at highest dosage level. No signs in the other groups.	2500
	2000	2/6		
	1000	0/6		

Brief description of tests procedure: Each of the above compounds was suspended in a vehicle consisting of 20% Sesame oil in 0.2% Tween 800 and fed orally to male albino CF strain mice weighing 19-25 grams. The mice had been starved for approximately 18 hours prior to the tests. The LD₅₀'s were calculated graphically according to the method of Litchfield and Wilcoxon.

DI-t-BUTYL PEROXIDE

1. <u>Dose mg/kg.</u>	<u>Mortality</u>	<u>Toxicological Signs</u>	<u>LD₅₀ mg/kg.</u>
4000	1/6	Excitation and slight hyper-ventilation at the highest dosage levels.	4000
2000	1/6		
1000	0/6		

Brief description of test procedure: The above compound was suspended in a vehicle consisting of 20% Sesame oil in 0.2% Tween 800 and fed orally at graded dosage levels to male albino CF strain mice weighing 19-25 grams. The mice had been starved for approximately 18 hours prior to the tests. The LD₅₀'s were calculated graphically according to the method of Litchfield and Wilcoxon.

(This information was prepared by the Pharmaceutical Laboratory of Wallace & Tiernan, Inc. at Belleville, N.J.).

2. <u>Compound</u>	<u>LD₅₀</u>		<u>LC₅₀</u>		<u>Maximal Non-irritating Strength</u>	
	<u>mg Compound/kg Body Weight</u>		<u>ppm</u>		<u>% Peroxide in Vehicle</u>	
	<u>Intra-peritoneal Rats</u>	<u>Oral (Gavage) Rats</u>	<u>Inhalation Rats</u>	<u>Mice</u>	<u>Skin Rabbits</u>	<u>Eye Rabbits</u>
Di-t-Butyl Peroxide (ROOR)	3210	>25000	>4103	>4103	97	97

Rats exposed to di-t-butyl peroxide vapor (4103 ppm) developed head and neck tremors uniformly in all six rats after ten minutes of exposure. A weakness in the extremities occurred, appearing first in the forelegs, later in the hindlegs. After 45 minutes the tremors lessened in all the rats. After 1 hour and 45 minutes one of the rats showed signs of hyperactivity at 10-second intervals. At the end of the 4-hour exposure the tremors had virtually disappeared, and the rats remained prostrate. Seven days later the hyperactive rat died: the only death of the six exposed rats.

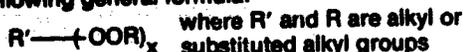
The mice were less affected than the rats, exhibiting only excitability and somewhat labored breathing. This occurred after ten minutes of exposure, was maximal at 30 to 50 minutes, and still persisted, though somewhat lessened at the end of the exposure period. The high dosage levels of each of the peroxides tested by the inhalation route caused prophyrin deposition in the nostrils and irregular respiration in the majority of the rats and mice.

(Reprinted from American Industrial Hygiene Assoc. Journal, 12, #3, June 1958).

DIALKYL PEROXIDES

INTRODUCTION

Dialkyl peroxides are organic compounds that have the following general formula:

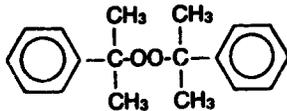


Di-tertiary alkyl peroxides are among the most stable of all the commercially available organic peroxides.

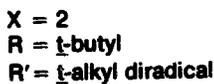
For the most common monofunctional di-tertiary alkyl peroxides;



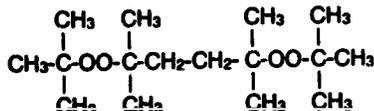
such as Luperox 500,



For the most common difunctional di-tertiary alkyl peroxides;



such as Lupersol 101,



The free radicals generated from dialkyl peroxide decomposition are efficient for **crosslinking** polyolefins (polyethylene and ethylene-vinyl acetate); **vulcanizing agents** for elastomers (ethylene propylene copolymers and terpolymers); **curing agents** for polyester resins; **initiators** in bulk, and suspension vinyl polymerizations and as **synergists** for flame retardant polymers.

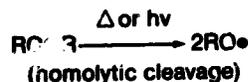
COMMERCIAL DIALKYL PEROXIDES

Typical physical and chemical properties of commercially available di-tertiary alkyl peroxides are enclosed. For greater convenience in handling and storage, some are available on an inert filler.

REACTIONS OF DIALKYL PEROXIDES

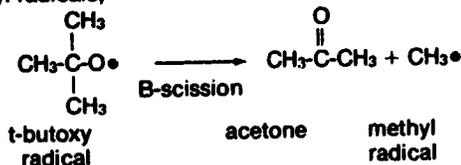
Primary Reaction

When subjected to heat or irradiation, dialkyl peroxides decompose homolytically into two free radicals;



Secondary Reaction

Tertiary alkoxy radicals can undergo further fragmentation (e.g. B-scission) to form ketones and alkyl radicals;

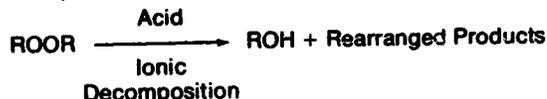


Radicals produced by either primary or secondary reactions initiate the desired free radical reaction.

Acid or Base Hydrolysis-Ionic Decomposition

In the presence of strong bases, di-tertiary alkyl peroxides are unattacked.

In the presence of strong oxidizing agents, reducing agents and accelerators (cobalt naphthenate or dimethylaniline) di-tertiary alkyl peroxides can decompose ionically forming non-radical products. Such products do not initiate free radical reactions.



Decomposition Products

The decomposition kinetics of dialkyl peroxides in dilute benzene solutions are first order. Similar behavior has been observed in a polymer matrix.¹ In both cases, the rate determining step appears to be the homolytic cleavage of the oxygen-oxygen bond (primary reaction).

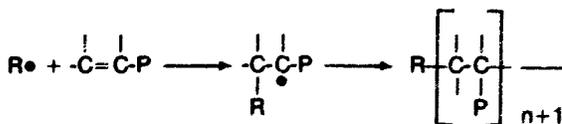
The chemical nature of the radicals depend upon their environment. For example:

In the presence of ABSTRACTABLE HYDROGENS on a polymer they can abstract hydrogen forming new polymer radicals which can then combine to form a crosslink bond.



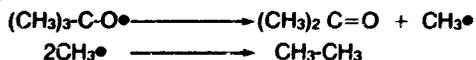
In the presence of other reactive species in a polymer, such as DOUBLE BONDS, the radicals can also react via addition-type reaction forming different polymer radicals, which can combine or react with additional such polymers to form multiple cross-link bonds.

(1) G.A. Harpell & D.H. Walrod, *Rubber Chem. & Tech.*, Vol. 46 No. 4 Sept. 1973, "Organic Peroxides for Cure of Ethylene-Propylene Rubbers."



Crosslinked polymer or
polymerized monomer

In a gas phase or in an inert media, the radicals will decompose forming ketones, alkanes and alkenes. e.g.:



Typical decomposition products of dialkyl peroxides in inert medias are included in the physical characteristics section for each peroxide.

STORAGE AND HANDLING

Facilities

Dialkyl peroxides should be stored in a cool (<100°F) place, separated from the manufacturing area, away from other combustible materials, and in accordance with the labeling designed for each specific package. Storage buildings should be well ventilated.

Storage Temperatures

To minimize evaporation and loss of active oxygen, dialkyl peroxides should be stored below 100°F.

HANDLING PRECAUTIONS

Containers (other than Liqua-Bins)

Dialkyl peroxides should be stored in their original container. Drain containers completely and flush with a suitable solvent, such as odorless mineral spirits, before discarding. Render the containers non-usable. Never allow residual peroxide to remain undiluted in discarded containers.

LIQUA-BIN CONTAINERS

This 3500 pound (net), 450 gallon container is a stainless steel package designed for repeated use. Specific handling and use information is available upon request. (Liqua-Bin containers used for Luperox 500T and Luperox 500R product packaging only.)

Materials of Construction — Materials of construction in contact with dialkyl peroxides should generally be limited to inert materials like polyethylene, Teflon, Nylon and Kel-F, reinforced plastics, Type 304 and 316 stainless steel or Tantalum.

Flammability — Di-t-butyl peroxide has a low flow point and its vapors are highly flammable, thus it must be handled as a Flammable Liquid. All other dialkyl peroxides have relatively high flash points, but once ignited, burn vigorously and are very difficult to extinguish. All dialkyl peroxides should be kept away from sources of heat and ignition such as radiators, steam pipes, direct rays of the sun, sparks and open flames.

Contamination — Care should be taken to avoid all forms of contamination with peroxides, particularly oxidizing and reducing agents and metal salts — "Especially strong mineral acids."

Static Electricity — When handling dialkyl peroxides, generally accepted methods of reducing static electricity, e.g.: grounding of equipment, shortening freefall of material, etc. are recommended.

FIRE

If a small fire occurs, class B type extinguishers (dry chemical foam or carbon dioxide) can be used. In case of a fire involving large quantities of dialkyl peroxides, the area should be evacuated and the fire fought with water spray or foam.

SPILLAGE AND DISPOSAL

Small Quantities — If a small quantity of a dialkyl peroxide is spilled, an inert absorbent material, such as vermiculite, should be used to soak up (liquids) or dilute the solid peroxide. The sweepings can then be disposed of by burning in a remote area.

Large Quantities — Larger quantities of dialkyl peroxides should be diluted to less than 1% active oxygen or less than 10% assay, whichever is lower with kerosene or Fuel Oil #2 and subsequently burned in a suitable furnace or incinerator. Provisions must be made for introducing the dilute peroxide solution into the furnace or incinerator as slowly as practicable. Dialkyl peroxides burned under these conditions will emit less air pollutants into the atmosphere since the peroxide is destroyed completely and effectively.

The above procedures should not be employed in violation of Federal, State or Local regulations.

TOXICITY

All the physiological effects have not been determined for dialkyl peroxides. In general, dialkyl peroxides should be considered mild skin and eye irritants. The following data has been reported:

Dialkyl Peroxide	Eye Irritation	Skin Irritation	Acute Oral Toxicity LD ₅₀ in Rats	Mutagenicity Ames Test
Di-t-butyl peroxide	slight	slight	>25,000 mg/kg	Negative
Luperox 500	slight	mild	4100 mg/kg	Negative
Lupersol 101	slight	slight	3200 mg/kg	—
Lupersol 130	slight	slight	1850 mg/kg*	—
Lupersol 801	slight	severe	5.18 ml/kg**	Negative

* value listed represents acute intraperitoneal toxicity LD₅₀ in mice.

** (— 4895 mg/kg)

FIRST AID

Care should be exercised by all personnel handling dialkyl peroxides. Do not allow prolonged contact with skin. Inhalation of vapors or decomposition products emitted during processing should be avoided.

In case of skin or eye contact with a dialkyl peroxide or its decomposition products, wash skin with plenty of soap and water, immediately flush eyes with water for at least 15 minutes and get medical attention. If swallowed, do not induce vomiting, call a physician.

(Continued on back cover)

PHYSICAL PROPERTIES OF DIALKYL PEROXIDES

SPECIFICATIONS

Commercial Product	Dialkyl Peroxide Structure Molecular Weight	Assay (%)	Active Oxygen (%)	Form	Filler	Melting-Freezing Point(s), °C
Lupersol 101	2,5-dimethyl-2,5-bis-(t-butylperoxy)hexane $\begin{array}{c} \text{CH}_3 \quad \text{CH}_3 \\ \quad \\ (\text{CH}_3)_3\text{COO}-\text{C}-\text{CH}_2-\text{CH}_2-\text{C}-\text{OOC}(\text{CH}_3)_3 \\ \quad \\ \text{CH}_3 \quad \text{CH}_3 \end{array}$	90.0 min.	9.92 min.	Liquid	—	Below 8°
Luperco 101-XL	M.W. 290.45	45.0-48.0	4.96-5.29	Free Flowing Powder	CaCO ₃	—
Lupersol 130	2,5-dimethyl-2,5-bis-(t-butylperoxy)hexyne-3 $\begin{array}{c} \text{CH}_3 \quad \text{CH}_3 \\ \quad \\ (\text{CH}_3)_3\text{COO}-\text{C}-\text{C} \equiv \text{C}-\text{C}-\text{OOC}(\text{CH}_3)_3 \\ \quad \\ \text{CH}_3 \quad \text{CH}_3 \end{array}$	90.0-95.0	10.05-10.61	Liquid	—	Below 8°
Luperco 130-XL	M.W. 286.42	45.0 min.	5.03 min.	Free Flowing Powder	CaCO ₃	—
Luperox 500T (Technical)	DICUMYL PEROXIDE $\begin{array}{c} \text{CH}_3 \quad \text{CH}_3 \\ \quad \\ \text{C}-\text{OO}-\text{C} \\ \quad \\ \text{CH}_3 \quad \text{CH}_3 \end{array}$	91.0 min.	5.40	Semi-crystalline Solid @ 25°C	—	30°
Luperox 500R (Recrystallized)		99 min.	5.87 min.	Crystalline Solid @ 25°C	—	38°
Luperco 500-40C		39.5-41.5	2.34-2.46	Free Flowing Powder	CaCO ₃	—
Luperco 500-40KE		39.5-41.5	2.31-2.46	Free Flowing Powder	Burgess KE Clay	—
Di-t-Butyl Peroxide	$\begin{array}{c} \text{CH}_3 \quad \text{CH}_3 \\ \quad \\ \text{CH}_2-\text{C}-\text{OO}-\text{C}-\text{CH}_3 \\ \quad \\ \text{CH}_3 \quad \text{CH}_3 \end{array}$ M.W. 146.22	98.5 min.	10.8 min.	Liquid	—	Below -40°
Lupersol 801	$\begin{array}{c} \text{CH}_3 \quad \text{CH}_3 \\ \quad \\ \text{CH}_2-\text{C}-\text{OO}-\text{C}-\text{C}_6\text{H}_5 \\ \quad \\ \text{CH}_3 \quad \text{CH}_3 \end{array}$ M.W. 208.29	90.0-95.0	6.91-7.30	Liquid	—	-0°

(1) Self accelerating decomposition temperature, A.S.T.M./UN Method

Table
 Dispensing
 Products
 in
 Metric Media

	0.8850 min. @ 25°	1.4180 min. @ 25°	115°/10.0 158°/55.0 249°/760	100°(38°)	86° 30# Cube	110°(43°)	Methane Ethane Ethylene Acetone t-Butyl Alcohol
	1.248 gm/cc @ 25° or 38.5 lbs./cu.ft. (loose) @ 25°	—	—	100°(38°)	82° 100# Drum	—	
	0.886-0.890 @ 25°	1.4260-1.4300 @ 25°	113°/10.0 151°/55.0 243°/760	100°(38°)	93° 35# Cube	188°(87°)	Methane Ethane Carbon Monoxide Carbon Dioxide Acetone t-Butyl Alcohol
	1.263 gms/cc @ 25° or 44 lbs./cu.ft. @ 25°	—	—	100°(38°)	88° 100# Drum	—	
	0.997-1.009 @ 40°	1.5279-1.5295 @ 43°	—	100°(38°)	91° 40# Pail	>200°(>93°)	
	1.00 @ 40°	1.5280 @ 43°	—	100°(38°)	—	>200°(>93°)	Methane Acetophenone Cumyl Alcohol
	1.611 gms/cm ³ @ 25° or 30 lbs./cu.ft. 40°	—	—	100°(38°)	—	—	
	1.579 gm/cm ³ @ 25° or 30 lbs./cu.ft. @ 40°	—	—	100°(38°)	—	—	
	0.785-0.790 @ 25°	1.3850-1.3900 @ 25°	10°/10.0 40°/55.0 111°/760	100°(38°)	80° 30# Cube	<76°(<24°)	Acetone t-Butyl Alcohol
	0.945 @ 25°	1.4819 @ 20°	—	100°(38°)	>80° 7# Bottle	174°(79°)	Methane Acetone Acetophenone Cumyl Alcohol

STORAGE, PACKAGING AND SHIPPING INFORMATION

Commercial Product	Maximum Storage Temp. F./C.	C.A.S. Registry Number	Container Shipping C/N	Net Weight	DOT Description, Hazard Class, Labeling, DOT Label
Lupersol 101	100°(38°)	76-63-7	30 gal. P.E. lined steel drum 5 gal. P.E. bottle 4 x 1 gal. P.E. bottle	200 lbs. 35 lbs. 4 x 7 lbs.	2,5-Dimethyl-2,5-Di(tert-butylperoxy) hexane Organic Peroxide "Organic Peroxide" Label
Luperco 101-XL	100°(38°)	76-63-7 471-34-1	Fiberdrum Fiberdrum	25 lbs. 100 lbs.	Nonregulated
Lupersol 130	100°(38°)	1068-27-5	5 gal. P.E. bottle 4 x 1 gal. P.E. bottle	35 lbs. 4 x 7 lbs.	2,5-Dimethyl-2,5-di(tert-butylperoxy) hexyne-3 Organic Peroxide "Organic Peroxide" Label
Luperco 130-XL	100°(38°)	1068-27-5 471-34-1	Fiberdrum	25 lbs.	Nonregulated
Luperox 500T (Technical)	100°(38°)	80-43-3	455 gal. liqua-bin 55 gal. steel drum 5 gal. HDPE ⁽³⁾ pail	3500 lbs. 425 lbs. 40 lbs.	Dicumyl Peroxide Organic Peroxide "Organic Peroxide" Label
Luperox 500R (Recrystallized)	100°(38°)	80-43-3	455 gal. liqua-bin 55 gal. steel drum 5 gal. HDPE ⁽³⁾ pail	3500 lbs. 275 lbs. 25 lbs.	Dicumyl Peroxide Organic Peroxide "Organic Peroxide" Label
Luperco 500-40C	100°(38°)	80-43-3 471-34-1	Fiberdrum Cor. Carton	25 lbs. 100 lbs.	Nonregulated
Luperco 500-40KE	100°(38°)	80-43-3 12141-46-7	Fiberdrum Cor. Carton	25 lbs. 100 lbs.	Nonregulated
Di-tert-Butyl Peroxide	100°(38°)	110-0504	55 gal. steel drum 15 gal. steel drum 5 gal. P.E. bottles 4 x 1 gal. P.E. bottle	340 lbs. 100 lbs. 30 lbs. 4 x 6 lbs.	Di-tert-Butyl Peroxide Flammable Liquid "Flammable Liquid" and "Organic Peroxide" Labels
Lupersol 801	100°(38°)	3457-61-2	55 gal. steel drum 4 x 1 gal. P.E. bottle	400 lbs. 4 x 7 lbs.	Tert-butyl cumyl peroxide Organic Peroxide "Organic Peroxide" Label

(2) Other containers are available on request
(3) High density polyethylene

	X		X	X	X			6.52	—	3.37	Lupersol 101 is completely miscible in most organic solvents.	INS
			X	X	X			—	—	—	Note: Luperco 101-XL contains calcium carbonate as filler.	
	X		X	X	X		X	7.4	5.0	3.6	Lupersol 130 is completely miscible in most organic solvents.	INS
			X	X	X		X	—	—	—	Note: Luperco 130-XL contains calcium carbonate as filler.	
	X		X	X	X			—	—	SEMI SOLID	Luperox 500R and Luperox 500T are very soluble (50-99%) in most organic solvents. Solubility in low molecular weight alcohols may be less than 50%. Note: Luperco 500-40C contains calcium carbonate as filler. Luperco 500-40KE contains Burgess KE clay as filler.	INS
	X		X	X	X			—	—	SEMI SOLID		INS
			X	X	X			—	—	—		
			X	X	X			—	—	—		
	X		X	X	X		X	.85	.71	.63	Di-t-Butyl Peroxide is completely miscible in most organic solvents.	INS
	X		X	X	X		X	4.66	3.57	2.70	Lupersol 801 is completely miscible in most organic solvents.	INS

INS = Insoluble

AVAILABILITY

Lucidol manufactures dialkyl peroxides at its plants in Geneseo, New York and Crosby, Texas, servicing the U.S. and Canada and major ports and border crossings for export.

For additional information on prices or to place an order, contact the Sales Department:

Lucidol Division
Pennwalt Corporation
1740 Military Road
Buffalo, New York 14240
(716) 877-1740

TECHNICAL INFORMATION

The dialkyl peroxides are only one of the many classes of organic peroxides manufactured by Lucidol. Product bulletins are available for:

Diacyl Peroxides
Ketone Peroxides
Peroxydicarbonates
Peroxyesters
Tertiary Alkyl Hydroperoxides
Sulfonyl Peroxides
Peroxyketals

More detailed information on the use and handling of organic peroxides is contained in technical bulletins:

1. Bulletin 30.30, "Evaluation of Organic Peroxides From Half-Life Data"
2. Bulletin 30.43, "Safe Handling Storage and Transportation of Peroxides Requiring Refrigeration"

3. Bulletin 30.90, "Free Radical Initiators for the Suspension Polymerization of Vinyl Chloride"
4. Bulletin 16.1274 "Chemical Curing of Elastomers and Crosslinking of Thermoplastics"
5. Bulletin, "Organic Peroxides for Rubber Crosslinking . . . Including New Peroxide Curing Systems"
6. Bulletin, "Lower Temperature Organic Peroxide Crosslinking Agents"

Also available for loan are a number of safety films tailored for various audiences.

FOOD AND DRUG ADMINISTRATION STATUS

The following dialkyl peroxides are listed in the Code of Federal Regulations; Title 21 "Food and Drugs" part 170 under "Food Additives,"

<u>Dialkyl Peroxide</u>	<u>Applicable Paragraphs</u>
Di-t-butyl peroxide	176.170, 177.2600
Luperox 500	175.300, 175.105
	177.2600, 177.2420
Lupersol 101	177.2600

For literature, films, additional technical information or evaluation samples, contact the Marketing Services Department.

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"Pennwalt does not guarantee the correctness or accuracy of the information contained herein and Pennwalt shall assume no liability arising out of its use. The user should thoroughly test any application before commercialization. Our recommendations should not be taken as inducement to infringe any patent or violate any law, safety code or insurance regulations."

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LUCIDOL
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CHEMICALS • EQUIPMENT
HEALTH PRODUCTS

Revised 9/82
Reprinted 5/83

Litho U.S.A.

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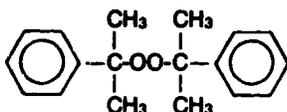


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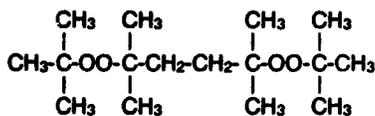
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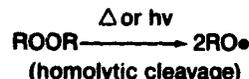
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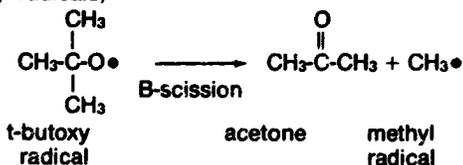
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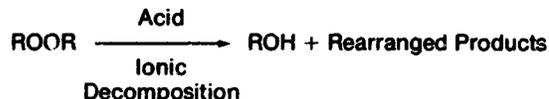


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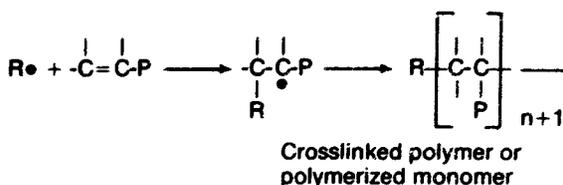
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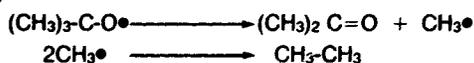


In the presence of other reactive species in a polymer, such as **DOUBLE BONDS**, the radicals can also react via addition-type reaction forming different polymer radicals, which can combine or react with additional such polymers to form multiple cross-link bonds.

(1) G.A. Harpell & D.H. Walrod, *Rubber Chem. & Tech.*, Vol. 46 No. 4 Sept. 1973, "Organic Peroxides for Cure of Ethylene-Propylene Rubbers."



In a gas phase or in an inert media, the radicals will decompose forming ketones, alkanes and alkenes. e.g.:



Typical decomposition products of dialkyl peroxides in inert medias are included in the physical characteristics section for each peroxide.

STORAGE AND HANDLING

Facilities

Dialkyl peroxides should be stored in a cool (<100°F) place, separated from the manufacturing area, away from other combustible materials, and in accordance with the labeling designed for each specific package. Storage buildings should be well ventilated.

Storage Temperatures

To minimize evaporation and loss of active oxygen, dialkyl peroxides should be stored below 100°F.

HANDLING PRECAUTIONS

Containers (other than Liqua-Bins)

Dialkyl peroxides should be stored in their original container. Drain containers completely and flush with a suitable solvent, such as odorless mineral spirits, before discarding. Render the containers non-usable. Never allow residual peroxide to remain undiluted in discarded containers.

LIQUA-BIN CONTAINERS

This 3500 pound (net), 450 gallon container is a stainless steel package designed for repeated use. Specific handling and use information is available upon request. (Liqua-Bin containers used for Luperox 500T and Luperox 500R product packaging only.)

Materials of Construction — Materials of construction in contact with dialkyl peroxides should generally be limited to inert materials like polyethylene, Teflon, Nylon and Kel-F, reinforced plastics, Type 304 and 316 stainless steel or Tantalum.

Flammability — Di-t-butyl peroxide has a low flow point and its vapors are highly flammable, thus it must be handled as a Flammable Liquid. All other dialkyl peroxides have relatively high flash points, but once ignited, burn vigorously and are very difficult to extinguish. All dialkyl peroxides should be kept away from sources of heat and ignition such as radiators, steam pipes, direct rays of the sun, sparks and open flames.

Contamination — Care should be taken to avoid all forms of contamination with peroxides, particularly oxidizing and reducing agents and metal salts - "Especially strong mineral acids."

Static Electricity — When handling dialkyl peroxides, generally accepted methods of reducing static electricity, e.g.: grounding of equipment, shortening freefall of material, etc. are recommended.

FIRE

If a small fire occurs, class B type extinguishers (dry chemical foam or carbon dioxide) can be used. In case of a fire involving large quantities of dialkyl peroxides, the area should be evacuated and the fire fought with water spray or foam.

SPILLAGE AND DISPOSAL

Small Quantities — If a small quantity of a dialkyl peroxide is spilled, an inert absorbent material, such as vermiculite, should be used to soak up (liquids) or dilute the solid peroxide. The sweepings can then be disposed of by burning in a remote area.

Large Quantities — Larger quantities of dialkyl peroxides should be diluted to less than 1% active oxygen or less than 10% assay, whichever is lower with kerosene or Fuel Oil #2 and subsequently burned in a suitable furnace or incinerator. Provisions must be made for introducing the dilute peroxide solution into the furnace or incinerator as slowly as practicable. Dialkyl peroxides burned under these conditions will emit less air pollutants into the atmosphere since the peroxide is destroyed completely and effectively.

The above procedures should not be employed if in violation of Federal, State or Local regulations.

TOXICITY

All the physiological effects have not been determined for dialkyl peroxides. In general, dialkyl peroxides should be considered mild skin and eye irritants. The following data has been reported:

Dialkyl Peroxide	Eye Irritation	Skin Irritation	Acute Oral Toxicity LD ₅₀ in Rats	Mutagenicity Ames Test
Di-t-butyl peroxide	slight	slight	>25,000 mg/kg	Negative
Luperox 500	slight	mild	4100 mg/kg	Negative
Lupersol 101	slight	slight	3200 mg/kg	—
Lupersol 130	slight	slight	1850 mg/kg*	—
Lupersol 801	slight	severe	5.18 ml/kg**	Negative

*Value listed represents acute intraperitoneal toxicity LD₅₀ in mice.

** (- 4895 mg/kg)

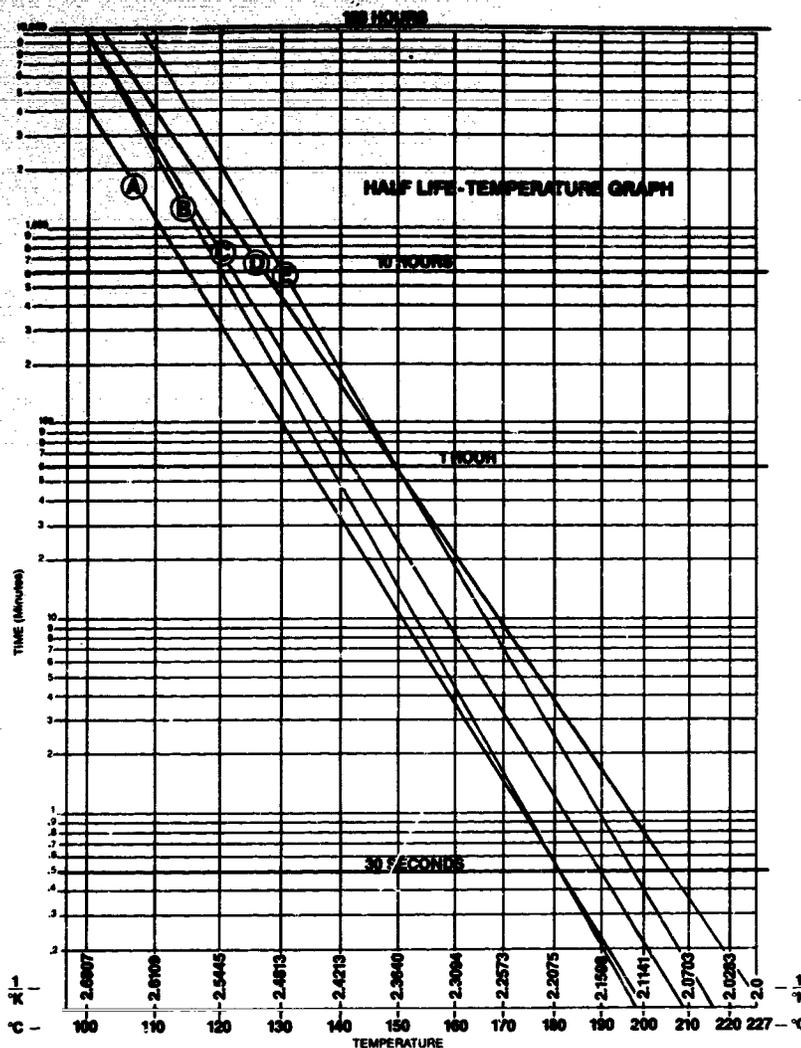
FIRST AID

Care should be exercised by all personnel handling dialkyl peroxides. Do not allow prolonged contact with skin. Inhalation of vapors or decomposition products emitted during processing should be avoided.

In case of skin or eye contact with a dialkyl peroxide or its decomposition products, wash skin with plenty of soap and water, immediately flush eyes with water for at least 15 minutes and get medical attention. If swallowed, do not induce vomiting, call a physician.

(Continued on back cover.)

0124



- A. Dicumyl Peroxide (LUPEROX 500R)
- B. 2,5-Dimethyl-2,5-Di(t-Butylperoxy) Hexane (LUPERSOL 101)
- C. t-Butyl Cumyl Peroxide (LUPERSOL 801)
- D. 2,5-Dimethyl-2,5-Di(t-Butylperoxy) Hexyne-3 (LUPERSOL 130)
- E. DI-T-BUTYL PEROXIDE

Product Name	Chemical Name	Chemical Structure	Concentration	Temp. (°C)	t _{1/2} (Hours)	k ₁ (First Order Rate Constant)	ΔE Activation Energy (KCAL/MOL)	50% Half-life Temp. (°C)	10% Half-life Temp. (°C)
A. Luperox 500R	Dicumyl Peroxide	<chem>CC(C)(C)OC(=O)OC(C)(C)C1=CC=CC=C1</chem>	0.2M (Benzene)	130 145	1.8 0.28	0.377 2.47	38	136	116
B. Lupersol 101	2,5-Dimethyl-2,5-di(t-butylperoxy) hexane	<chem>CC(C)C(C)OC(=O)OC(C)(C)C</chem>	0.1M (Benzene)	115 130 145	17 2.3 0.40	0.042 0.247 1.71	40	138	119
C. Lupersol 801	t-Butyl Cumyl Peroxide	<chem>CC(C)(C)OC(=O)OC(C)(C)C1=CC=CC=C1</chem>	0.2M (Benzene)	115	17.2	0.040	36	142	121
D. Lupersol 130	2,5-Dimethyl-2,5-di(t-butylperoxy) hexyne-3	<chem>CC(C)C(C)OC(=O)OC(C)(C)C#C</chem>	0.1M (Benzene)	115 130 145 160	49 8.2 1.7 0.31	0.014 0.084 0.410 2.22	38	149	128
E. Di-t-Butyl Peroxide	Di-t-Butyl Peroxide	<chem>CC(C)(C)OC(=O)OC(C)(C)C</chem>	0.2M (Benzene)	100 115 130	220 34 6.4	0.003 0.020 0.018	36	149	128

NOTE: Half life values in polymers may differ.

0125

PHYSICAL PROPERTIES OF D-ALKYL PEROXIDES

SPECIFICATIONS

Commercial Product	D-alkyl Peroxide Structure Molecular Weight	Assay (%)	Active Oxygen (%)	Form	Filler	Melting Point (°C)	Freezing Point (°C)
Lupersol 101	2,5-dimethyl-2,5-bis-(t-butylperoxy)hexane $\begin{array}{c} \text{CH}_3 \quad \text{CH}_3 \\ \quad \\ (\text{CH}_3)_3\text{COO}-\text{C}-\text{CH}_2-\text{CH}_2-\text{C}-\text{OOC}(\text{CH}_3)_3 \\ \quad \\ \text{CH}_3 \quad \text{CH}_3 \end{array}$ M.W. 290.45	90.0 min.	9.92 min.	Liquid	—	Below 8°	
Luperco 101-XL		45.0-48.0	4.96-5.29	Free Flowing Powder	CaCO ₃	—	
Lupersol 130	2,5-dimethyl-2,5-bis-(t-butylperoxy)hexyne-3 $\begin{array}{c} \text{CH}_3 \quad \text{CH}_3 \\ \quad \\ (\text{CH}_3)_3\text{COO}-\text{C}-\text{C} \equiv \text{C}-\text{C}-\text{OOC}(\text{CH}_3)_3 \\ \quad \\ \text{CH}_3 \quad \text{CH}_3 \end{array}$ M.W. 286.42	90.0-95.0	10.05-10.61	Liquid	—	Below 8°	
Luperco 130-XL		45.0 min.	5.03 min.	Free Flowing Powder	CaCO ₃	—	
Luperox 500T (Technical)	DICUMYL PEROXIDE $\begin{array}{c} \text{CH}_3 \quad \text{CH}_3 \\ \quad \\ \text{C}_6\text{H}_5-\text{C}-\text{OO}-\text{C}-\text{C}_6\text{H}_5 \\ \quad \\ \text{CH}_3 \quad \text{CH}_3 \end{array}$ M.W. 270.37	91.0 min.	5.40	Semi-crystalline Solid @ 25°C	—	30°	
Luperox 500R (Recrystallized)		99 min.	5.87 min.	Crystalline Solid @ 25°C	—	38°	
Luperco 500-40C		39.5-41.5	2.34-2.46	Free Flowing Powder	CaCO ₃	—	
Luperco 500-40KE		39.5-41.5	2.34-2.46	Free Flowing Powder	Burgess KE Clay	—	
Di-t-Butyl Peroxide	$\begin{array}{c} \text{CH}_3 \quad \text{CH}_3 \\ \quad \\ \text{CH}_3-\text{C}-\text{OO}-\text{C}-\text{CH}_3 \\ \quad \\ \text{CH}_3 \quad \text{CH}_3 \end{array}$ M.W. 146.22	98.5 min.	10.8 min.	Liquid	—	Below -40°	
Lupersol 801	$\begin{array}{c} \text{CH}_3 \quad \text{CH}_3 \\ \quad \\ \text{CH}_3-\text{C}-\text{OO}-\text{C}-\text{C}_6\text{H}_5 \\ \quad \\ \text{CH}_3 \quad \text{CH}_3 \end{array}$ M.W. 208.29	90.0-95.0	6.91-7.30	Liquid	—	-0°	

(1) Self accelerating decomposition temperature, A.S.T.M./UN Method

	0.8650 min. @ 25°	1.4160 min. @ 25°	115°/10.0 158°/55.0 249°/760	100°(38°)	86° 30# Cube	110°(43°)	Methane Ethane Ethylene Acetone t-Butyl Alcohol
	1.248 gm/cc @ 25° 38.5 lbs./cu.ft. (loose) @ 25°	—	—	100°(38°)	82° 100# Drum	—	
	0.886-0.890 @ 25°	1.4260-1.4300 @ 25°	113°/10.0 151°/55.0 243°/760	100°(38°)	93° 35# Cube	188°(87°)	Methane Ethane Carbon Monoxide Carbon Dioxide Acetone t-Butyl Alcohol
	1.263 gm/cc @ 25° or 44 lbs./cu.ft. @ 25°	—	—	100°(38°)	88° 100# Drum	—	
	0.997-1.009 @ 40°	1.5279-1.5295 @ 43°	—	100°(38°)	91° 40# Pail	>200°(>93°)	
	1.00 @ 40°	1.5280 @ 43°	—	100°(38°)	—	>200°(>93°)	Methane Acetophenone Cumyl Alcohol
	1.611 gm/cm ³ @ 25° or 30 lbs./cu.ft. 40°	—	—	100°(38°)	—	—	
	1.579 gm/cm ³ @ 25° or 30 lbs./cu.ft. @ 40°	—	—	100°(38°)	—	—	
	0.785-0.790 @ 25°	1.3850-1.3900 @ 25°	10°/10.0 40°/55.0 111°/760	100°(38°)	80° 30# Cube	<76°(<24°)	Acetone t-Butyl Alcohol
	0.945 @ 25°	1.4819 @ 20°	—	100°(38°)	>80° 7# Bottle	174°(79°)	Methane Acetone Acetophenone Cumyl Alcohol

STORAGE, PACKAGING AND SHIPPING INFORMATION

Commercial Product	Maximum Storage Temp. F./C.	C.A.S. Registry Number	Container / Shipping CTN	Net Weight	DOT Description / Hazard Classification / DOT Label
Lupersol 101	100°(38°)	78-63-7	30 gal. P.E. lined steel drum 5 gal. P.E. bottle 4 x 1 gal. P.E. bottle	200 lbs. 35 lbs. 4 x 7 lbs.	2,5-Dimethyl-2,5-di(tert-butylperoxy) hexane Organic Peroxide "Organic Peroxide" Label
Luperco 101-XL	100°(38°)	78-63-7 471-34-1	Fiberdrum Fiberdrum	25 lbs. 100 lbs.	Nonregulated
Lupersol 130	100°(38°)	1068-27-5	5 gal. P.E. bottle 4 x 1 gal. P.E. bottle	35 lbs. 4 x 7 lbs.	2,5-Dimethyl-2,5-di(tert-butylperoxy) hexyne-3 Organic Peroxide "Organic Peroxide" Label
Luperco 130-XL	100°(38°)	1068-27-5 471-34-1	Fiberdrum	25 lbs.	Nonregulated
Luperox 500T (Technical)	100°(38°)	80-43-3	455 gal. liqua-bin 55 gal. steel drum 5 gal. HDPE ⁽³⁾ pail	3500 lbs. 425 lbs. 40 lbs.	Dicumyl Peroxide Organic Peroxide "Organic Peroxide" Label
Luperox 500R (Recrystallized)	100°(38°)	80-43-3	455 gal. liqua-bin 55 gal. steel drum 5 gal. HDPE ⁽³⁾ pail	3500 lbs. 275 lbs. 25 lbs.	Dicumyl Peroxide Organic Peroxide "Organic Peroxide" Label
Luperco 500-40C	100°(38°)	80-43-3 471-34-1	Fiberdrum Cor. Carton	25 lbs. 100 lbs.	Nonregulated
Luperco 500-40KE	100°(38°)	80-43-3 121-41-46-7	Fiberdrum Cor. Carton	25 lbs. 100 lbs.	Nonregulated
Di-t-Butyl Peroxide	100°(38°)	110-0504	55 gal. steel drum 15 gal. steel drum 5 gal. P.E. bottles 4 x 1 gal. P.E. bottle	340 lbs. 100 lbs. 30 lbs. 4 x 6 lbs.	Di-tert-Butyl Peroxide Flammable Liquid "Flammable Liquid" and "Organic Peroxide" Labels
Lupersol 801	100°(38°)	3457-61-2	55 gal. steel drum 4 x 1 gal. P.E. bottle	400 lbs. 4 x 7 lbs.	Tert-butyl cumyl peroxide Organic Peroxide "Organic Peroxide" Label

(2) Other containers are available on request
(3) High density polyethylene

	X		X	X	X			6.52	—	3.37	Lupersol 101 is completely miscible in most organic solvents.	INS
			X	X	X			—	—	—	Note: Luperco 101-XL contains calcium carbonate as filler.	
	X		X	X	X		X	7.4	5.0	3.6	Lupersol 130 is completely miscible in most organic solvents.	INS
			X	X	X		X	—	—	—	Note: Luperco 130-XL contains calcium carbonate as filler.	
	X		X	X	X			—	—	SEMI SOLID	Luperox 500R and Luperox 500T are very soluble (50-99%) in most organic solvents. Solubility in low molecular weight alcohols may be less than 50%. Note: Luperco 500-40C contains calcium carbonate as filler. Luperco 500-40KE contains Burgess KE clay as filler.	INS
	X		X	X	X			—	—	SEMI SOLID		INS
			X	X	X			—	—	—		
			X	X	X			—	—	—		
	X		X	X	X		X	.85	.71	.63	Di-t-Butyl Peroxide is completely miscible in most organic solvents.	INS
	X		X	X	X		X	4.66	3.57	2.70	Lupersol 801 is completely miscible in most organic solvents.	INS

INS = Insoluble

AVAILABILITY

Lucidol manufactures dialkyl peroxides at its plants in Geneseo, New York and Crosby, Texas, servicing the U.S. and Canada and major ports and border crossings for export.

For additional information on prices or to place an order, contact the Sales Department:

Lucidol Division
Pennwalt Corporation
1740 Military Road
Buffalo, New York 14240
(716) 877-1740

TECHNICAL INFORMATION

The dialkyl peroxides are only one of the many classes of organic peroxides manufactured by Lucidol. Product bulletins are available for;

Diacyl Peroxides
Ketone Peroxides
Peroxydicarbonates
Peroxyesters
Tertiary Alkyl Hydroperoxides
Sulfonyl Peroxides
Peroxyketals

More detailed information on the use and handling of organic peroxides is contained in technical bulletins;

1. Bulletin 30.30, "Evaluation of Organic Peroxides From Half-Life Data"
2. Bulletin 30.43, "Safe Handling, Storage and Transportation of Peroxides Requiring Refrigeration"

3. Bulletin 30.90, "Free Radical Initiators for the Suspension Polymerization of Vinyl Chloride"
4. Bulletin 16.1274 "Chemical Curing of Elastomers and Crosslinking of Thermoplastics"
5. Bulletin, "Organic Peroxides for Rubber Crosslinking . . . Including New Peroxide Curing Systems"
6. Bulletin, "Lower Temperature Organic Peroxide Crosslinking Agents"

Also available for loan are a number of safety films tailored for various audiences.

FOOD AND DRUG ADMINISTRATION STATUS

The following dialkyl peroxides are listed in the Code of Federal Regulations; Title 21 "Food and Drugs" part 170 under "Food Additives,"

<u>Dialkyl Peroxide</u>	<u>Applicable Paragraphs</u>
Di-t-butyl peroxide	176.170, 177.2600
Luperox 500	175.300, 175.105 177.2600, 177.2420
Lupersol 101	177.2600

For literature, films, additional technical information or evaluation samples, contact the Marketing Services Department.

For additional information contact the Marketing Services Department.

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HEALTH PRODUCTS

EFFECTS INFORMATION PROFILE

AUG 10 1983

ID No.	CHEMICAL NAME	SYNONYMS	CAS No.
74	Di-t-butyl peroxide		110-05-4

Description Clear, water-white liquid; may ignite organic materials or explode when shocked or in contact with reducing material.

Use Intermediate for ignition acceleator for diesel fuel, polymerization initiator, curing agent

Melting point: -40°C
 Vapor pressure (B.P.): 111°C
 Specific gravity: 0.791 (25/25 $^{\circ}\text{C}$)
 Water solubility: Insoluble
 Organic solubility: Soluble in styrene, ketones, most hydrocarbons
 Log P oct/water: 0.6
 Empirical formula: $\text{C}_8\text{H}_{18}\text{O}_2$

Structural Formula



Biochemical Information

Reference	Nature of Info.	Page

Observations in Humans

Reference	Nature of Info.	Page
Carson & Mumford (1978)	Industry hazards	6
Dautov (1977)	Hygiene	6

Environmental Information

Reference	Nature of Info.	Page
	Determination in air Thermal decomposition Effect on bacteria	7-8

Toxicological Information

Reference	Nature of Info.	Page
Vida et al. (1974)	Analgesics	5
Yamaguchi & Yamashita (1980)	Mutagenicity	5

Enclosures

Reference	Page
RTECS Clement (1978)	2-3 9-14

RTECS

YOU ARE NOW CONNECTED TO THE RTECS FILE. ✓
TOXICITY DATA IN NIOSH'S RTECS HAVE NOT BEEN CRITICALLY EVALUATED.
NP (')

SS 1 /C?
USER:
110-05-4
PROG:
SS (1) PSTG (1)

IP 94 ✓

RTECS

SS 2 /C?
USER:
PRT DL COMPLETE
PROG:

SI - NIOSH/ER2450000
N1 - t-BUTYL PEROXIDE
RN - 110-05-4
CC - TUMOR DATA
CC - PRIMARY IRRITANT
ST - REPORTED IN EPA TSCA INVENTORY, 1980
ST - MEETS CRITERIA FOR PROPOSED OSHA MEDICAL RECORDS RULE
FEREAC 47,30420,82
SY - CADOX
SY - DI-tert-BUTYLPEROXID (German)
SY - DI-t-BUTYL PEROXIDE
SY - DI-tert-BUTYL PEROXYDE (Dutch)
SY - DTBP
SY - PEROSSIDO DI BUTILE TERZIARIO (Italian)
SY - PEROXYDE DE BUTYLE TERTIAIRE (French)
MF - CS-H18-G2
MW - 146.26
WL - 1X1&1&00X1&1&1
EM - 7908
SO - AIHAAP American Industrial Hygiene Association Journal. 19,205,58
TDKW- SKIN;RABBIT;RODENTS;IRRITATION;500 mg
SO - 2BZPAK "Sbornik Vysledku Toxikologickeho Vysetreni Latek A
Pripravku," J.V. Marhold, Institut Pro Uchovu Vedoucich
Pracovniku Chemickeho Prumyclu Praha, Czechoslovakia, 1972
-,40,72
TDKW- EYE;RABBIT;RODENTS;IRRITATION;500 mg/24H ;TOXIC EFFECTS;MILD
CONTINUE PRINTING? (YES/NO)
USER:
YES
PROG:
SO - ZAARAM Zentralblatt fuer Arbeitsmedizin und Arbeitsschutz.
8,25,58
TDKW- EYE;RABBIT;RODENTS;IRRITATION;200 mg/1M rns ;TOXIC EFFECTS;MILD
SO - RARSAM Radiation Research, Supplement. 3,193,63
TDKW- UNKNOWN;MOUSE;RODENTS;TDLo;585 mg/kg;TOXIC EFFECTS;EQUIVOCAL
TUMORIGENIC AGENT
SO - AIHAAP American Industrial Hygiene Association Journal. 19,205,58
TDKW- INTRAPERITONEAL;RAT;RODENTS;LD50;3210 mg/kg;TOXIC EFFECTS
BEHAVIORAL SYMPTOMS

RTECS

SS 2 /C7

USER:

PRT TOXDATA COMPLETE

PROG:

SI - NIOSH/ER2450000

NI - t-BUTYL PEROXIDE

RI - 110-05-4

SO - AIHAAP American Industrial Hygiene Association Journal. 19,205,58

TDKW- SKIN;RABBIT;RODENTS;IRRITATION;500 mg

EO - 28ZPAK "Sbornik Vysledku Toxikologickeho Vysetreni Latek A
Pripravku," J.V. Marhold, Institut Pro Vychovu Vedoucich
Pracovniku Chemickeho Prumyслу Praha, Czechoslovakia, 1972
-40,72

TDKW- EYE;RABBIT;RODENTS;IRRITATION;500 mg/24H ;TOXIC EFFECTS;MILD

SO - ZAARAM Zentralblatt fuer Arbeitsmedizin und Arbeitsschutz.
8,25,58

TDKW- EYE;RABBIT;RODENTS;IRRITATION;200 mg/1M rns ;TOXIC EFFECTS;MILD

SO - RARSAM Radiation Research, Supplement. 3,193,63

TDKW- UNKNOWN;MOUSE;RODENTS;TDLo;585 mg/kg;TOXIC EFFECTS;EQUIVOCAL
TUMORIGENIC AGENT

SO - AIHAAP American Industrial Hygiene Association Journal. 19,205,58

TDKW- INTRAPERITONEAL;RAT;RODENTS;LD50;3210 mg/kg;TOXIC EFFECTS
BEHAVIORAL SYMPTOMS

SS 2 /C7

2

BIOCHEMICAL INFORMATION

- 7 SI - CA/898/849880X
 AU - Miyakawa T ; Takemoto LJ ; Fox CF
 AD - Mol. Biol. Inst., Univ. California, Los Angeles, Calif.
 TI - Membrane permeability of bifunctional, amino site-specific, cross-linking reagents
 SO - J. Supramol. Struct.; VOL 6, ISS 3, 1978,383-10
 LA - ENG
 CD - JSPMA
 AB - CBAC COPYRIGHT: CREN ABS The membrane permeability of a series of reversible cross-linking reagents which are diazide tartrate derivs. was compared with that of dimethyl 3,3'-dithiobispropionimidate-ZnCl (DTBP). (38285-78-8 dimethyl 3,3'-dithiobispropionimidate-ZnCl) The diazide tartrate derivs. tested included tartryldiazide (TDA), tartryldi(glycylazide) (TDGA), tartryldi(beta-alanylazide), tartryldi(gamma-aminobutyrylazide), and tartryldi(epsilon-aminocaproylazide) (TDCA). (54789-87-6 tartryldiazide)(54789-90-1 tartryldi(glycylazide))(68846-97-9 tartryldi(beta-alanylazide)(68846-98-0 tartryldi(gamma-aminobutyrylazide))(54789-92-2 tartryldi(epsilon-aminocaproylazide)) TDA, which has the shortest chain length of the diazide tartrate derivs. tested, was readily permeable through the erythrocyte membrane. When added at equal concns. to unsealed ghosts, TDGA was at least as reactive as DTBP in its ability to crosslink the internally displayed proteins 1, 2, 4.1, 4.2, and 6. Treatment of resealed ghosts by DTBP produced oligomeric complexes of these proteins plus apparent homo-oligomeric complexes of Hb. TDGA at the same concns. did not crosslink any of these components, indicating its membrane-impermeable nature. As the chain length of the homologous series increased from TDGA to TDCA, the crosslinkers became increasingly permeable through the erythrocyte membrane.
 RN - 38285-78-8; 54789-87-6; 54789-90-1; 68846-97-9; 68846-98-0;

- 8 SI - NEEP/80/12839
 AU - FIDLER JM ; NABER EC ; LATCHAM JD
 AD - Pennfield Corp., 721 Bohannon Rd., Lancaster, Pa. 17604, USA.
 TI - Effect of peroxide administration on selenium utilization, growth, deficiency symptoms, and glutathione peroxidase activity in chicks fed controlled selenium diets.
 SO - POULT SCI; 59 (1), 1980, 141-148.
 CD - POSCA
 AB - NEEP COPYRIGHT: BIOL ABS. The effect of peroxide administration on chick growth, severity of exudative diathesis and glutathione peroxidase activity was determined. Hydrogen peroxide reduced growth rate and usually reduced liver and plasma glutathione peroxidase activity. The severity of exudative diathesis was greatly influenced by dietary Se level but little if any relationship of this disease to peroxide-induced reductions in glutathione peroxidase activity was found. Neither ethoxyquin nor excess supplemental Se was effective in reversing the peroxide toxicity. The effect of hydrogen peroxide in reducing enzyme activity was related to decreased Se uptake and retention. Tertiary butyl peroxide administration caused a more serious depression in enzyme activity of liver than hydrogen peroxide. This organic peroxide caused a small, but non-significant, reduction in Se retention.
 RN - 7782-49-2; 110-05-4; 91-53-2
 EM - 8010

TOXICOLOGICAL INFORMATION

424

SI - CA/882/838478J
 AU - Vicks JA ; Samour CH ; O'Dea PM ; Mang TS T ; Rainhard JF
 AD - Kendall Co., Lexington, Mass.
 TI - Analgesics. 2. Selected 5-substituted
 5-(1-phenylethyl)barbituric acids
 SO - J. Med. Chem.; VOL 17, ISS 11, 1974,1194-7
 LA - ENG
 CD - JBCMA
 AB - CBAC COPYRIGHT: CHEM ABS Several title compds. showed better
 oral analgesic activity than codeine sulfate, and
 5-cyclopropylcarbonyloxy-5-(1-phenylethyl)barbituric acid (I) was
 about 18 times as potent s.c. as morphine sulfate in mice.
 (1428-83-7 Codeine sulfate)(53761-10-7
 5-Cyclopropylcarbonyloxy-5-(1-phenylethyl)barbituric
 acid)(64-31-3 Morphine sulfate) The compds. were also central
 nervous stimulants, and were devoid of hypnotic activity. I was
 prepd. from 5-(1-phenylethyl)barbituric acid by oxidn. to its
 5-hydroxy deriv. and esterification. (37555-98-9
 5-(1-Phenylethyl)barbituric acid)(37431-36-8
 5-Hydroxy-5-(1-phenylethyl)barbituric acid)
 RN - 1428-83-7; 53761-10-7; 64-31-3; 37555-98-9; 37431-36-8; 110-05-4;
 53761-12-2; 57-13-6; 37431-44-0; 53761-08-3; 37556-08-6;
 37555-99-0; 685-27-8; 53778-21-4; 53761-13-0; 37555-96-7;
 37555-95-6; 37431-38-2; 37431-37-1; 37431-39-3; 53761-09-4;
 585-71-7; 53761-11-8
 EN - 7812

Alif

SI - CA/893/143781H
 AU - Yamaguchi T ; Yamashita Y
 AD - Dep. Food Nutr., Yamaguchi Women's Univ., Yamaguchi
 TI - Mutagenicity of hydroperoxides of fatty acids and some
 hydrocarbons
 SO - Agric. Biol. Chem.; VOL 44, ISS 7, 1980,1675-8
 LA - ENG
 CD - ABCMA
 AB - CBAC COPYRIGHT: CHEM ABS The hydroperoxides of Na linoleate and
 Na linolenate were mutagenic to Salmonella typhimurium in the
 Ames mutagenicity test. Of the various types of hydrocarbon
 peroxides, only hydroperoxide type R-OOH showed mutagenicity,
 i.e., t-Bu hydroperoxide and cumene hydroperoxide, whereas
 dialkyl and diacyl peroxides showed no activity. (75-91-2
 tert-butyl hydroperoxide)(68-15-9 Cumene hydroperoxide) h202
 showed no mutagenicity.
 RN - 75-91-2; 68-15-9; 79-21-8; 68-43-3; 94-36-8; 185-74-8; 110-05-4;
 937-14-4; 7722-84-1; 11058-83-4; 75036-23-6
 EN - 8811

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OBSERVATIONS IN HUMANS

- 1 **SI** - HEEP/79/05342
AU - CARSON PA ; HILFORD CJ
AD - Unilever Res. Lab., Port Sunlight, Wirral, Merseyside L62 4XU, Cheshire, Engl., UK.
TI - Major hazards in the chemical industry: I. Their definition and significance.
SO - J OCCUP ACCID; 2 (1). 1978 1-24
CD - JOACD
AB - HEEP COPYRIGHT: BIOL ABS. The concept of major hazards to workers and the public and the background to the Advisory Committee on Major Hazards are outlined. Technical problems associated with defining major hazards and notifiable installations are discussed and some solutions proposed. Types of installations encompassed by the definition are identified.
- RN** - 24981-14-4; 10210-68-1; 10102-44-0; 10035-10-6; 10025-87-3; 9010-98-4; 9002-08-4; 9002-86-2; 8006-41-9; 8002-05-9; 7803-51-2; 7783-06-4; 7782-58-5; 7726-95-4; 7719-12-2; 7664-41-7; 7664-39-3; 7647-01-0; 7446-09-5; 2370-12-9; 929-06-6; 927-07-1; 762-12-9; 630-08-0; 629-11-8; 498-66-8; 302-01-2; 280-57-9; 150-76-5; 142-82-8; 135-19-3; 131-11-3; 124-89-4; 123-84-4; 123-72-8; 115-07-1; 111-65-9; 110-86-1; 110-85-0; 110-82-7; 110-54-3; 110-22-5; 110-15-6; 110-05-4; 109-66-0; 109-13-7; 108-95-2; 108-88-3; 107-71-1; 107-15-3; 107-13-1; 107-12-0; 106-98-9; 106-97-8; 106-42-3; 105-74-8; 105-64-6; 105-60-2; 105-08-8; 101-72-4; 100-74-3; 97-93-8; 96-22-0; 95-93-2; 94-36-0; 88-43-3; 80-15-9; 75-98-9; 75-91-2; 75-83-2; 75-44-5; 75-21-8; 74-98-6; 74-90-8; 74-85-1; 71-43-2; 67-56-1; 64-19-7; 64-17-5; 62-53-3; 60-29-7; 59-67-6; 57-14-7; 57-13-6
- EM** - 7905
- 2 **SI** - CA/088/065408A
AU - Dautov FF
AD - Kazan. Med. Inst. im. Kurashova, Kazan, USSR
TI - Hygienic characteristics of the working conditions in the production of organic peroxides
SO - Kazan. Med. Zh.; VOL 58, ISS 3, 1977,89-91
LA - RUS
CD - KAMZA
AB - CBAC COPYRIGHT: CHEM ABS Workers engaged in the prodn. of org. peroxides, s.g. tert-Bu perbenzoate and di-tert-Bu peroxide, suffered from gripe, angina, acute respiratory disease, pneumonia, and sound pollution. (614-45-9 tert-Butyl perbenzoate)(110-05-4 Di-tert-butyl peroxide) Working atms. were polluted by H₂O, H₂CO, H₂CH₂Cl, H₂S, tert-BuOH, H₂O₂, HCl, and the org. peroxides. (78-93-3 Methyl ethyl ketone)(100-44-7 Benzyl chloride)(75-65-0 tert-Butyl alcohol) Safety measures in the prodn. of org. peroxides are discussed.
- RN** - 614-45-9; 110-05-4; 78-93-3; 100-44-7; 75-65-0; 7647-01-0; 7664-41-7; 7722-84-1
- EM** - 7804

ENVIRONMENTAL INFORMATION

- Ex 1** SI - CA/992/8029130
 AU - Granditsch R ; Straichshier F ; Mankutti J
 AD - Vienna
 TI - Toxic effect of organic peroxides on bacterial flora of activated sludge and soil
 SO - Gesterr. Anzeiger-Rundsch., GBR Int.; VOL 24, ISS 6, 1979,99-101
 LA - GER
 CD - GARDIS
 AB - CBAC COPYRIGHT: CHEM ABS The toxic concns. of STBP, TBP, BP 99, CNP 99, and TBPB for activated sludge and soil microorganisms were 27.7, 0.29, 0.30, 0.0035, and 0.096 and >50, 0.1, 37, 0.1, and 0.0 wt.%, resp. (110-05-4 STBP)(75-91-2 TBP 80)(94-34-8 BP 99)(70-10-2 CNP 99)(66745-94-6 TBPB)
 RN - 110-05-4; 75-91-2; 94-34-8; 70-10-2; 66745-94-6
 EH - 8007
- 2** SI - CA/995/1926990
 AU - Ivanov KI ; Zager KE ; Kuz'mina MA ; Kulikovskaya TN
 AU - Tumanovskii AB ; Tamarkin LE ; Semanova MS ; Kon'shina GN
 TI - Removal of toxic impurities from the gas resulting from the combustion of power-plant fuels
 SO - U.S.S.R. PATENT NO. 841659 06/30/81 (All-Union Scientific-Research Thermotechnical Institute)
 LA - RUB
 AB - CBAC COPYRIGHT: CHEM ABS The degree of purifn. is increased by adding isopropylbenzene hydroperoxide or tert-Bu peroxide to flue gas. (88-15-9 Isopropylbenzene hydroperoxide)(110-05-4 tert-Butyl peroxide)
 RN - 88-15-9; 110-05-4
 EH - 8112
- Ex 2** SI - CA/994/8212644
 AU - Sapunkova GS ; Kulakova AS ; Yablokova AS
 AD - USSR
 TI - Determination of organic peroxides in the atmosphere of industrial buildings
 SO - Mater. Nauchno-Tekh. Konf. Kazan. Khim.-Tekhnol. Inst. Kazan. Zavoda Org. Sint., 2nd; 1973,157-9
 LA - RUSS
 CD - 3LIUA
 AB - CBAC COPYRIGHT: CHEM ABS Air (1-5 l.) was passed through an absorber contg. 3 ml ethylene glycol. The soln. was then mixed with 1 ml reagent (50 MeOH + 0.25 ml 6N H2SO4 satd. with Mohr's salt) and the color was detd. after 10 min vs. a blank. A linear calibration curve was obtained for 0-8.0 mug H2O2 and 0-14.0 mug methyl ethyl ketone peroxide, tert-Bu perbenzoate, tert-Bu hydroperoxide, lauroyl peroxide, or di-tert-Bu peroxide. (7722-84-1 Hydrogen peroxide)(1330-23-4 Methyl ethyl ketone peroxide)(614-45-9 tert-Butyl perbenzoate)(75-91-2 tert-Butyl hydroperoxide)(105-74-8 Lauroyl peroxide)(110-05-4 Di-tert-butyl peroxide)
 RN - 7722-84-1; 1330-23-4; 614-45-9; 75-91-2; 105-74-8; 110-05-4
 EH - 7612

ENVIRONMENTAL INFORMATION

- E-4 * SI - CA/008/1641608
 AU - Sawai T ; Sawai T
 AB - Tokyo Natrop. Isot. Res. Cent., Tokyo, Japan
 TI - Thermal decomposition of polychlorinated biphenyls (PCB) in alkaline 2-propanol solutions
 SO - Kagai; VOL 6, ISS 4, 1975,234-9
 LA - Japan
 CD - KSAIA
 AB - CSAC COPYRIGHT: CHEM ABS The dechlorination of polychlorinated biphenyls (PCB's) is accelerated by radicals generated from org. peroxides, e.g., di-tert-butyl peroxide (I). (110-05-4 Di-tert-butyl peroxide) For example, heating PCB's in alkaline 2-propanol soln. for 2 hr at 130.degree. almost completely decomposed the PCB's, forming biphenyl, KCl, tert-butanol, and acetone. (67-63-0 2-Propanol)(92-52-4 Biphenyl)(75-65-0 tert-Butanol)(67-64-1 Acetone) The dechlorination of PCB's by other radical initiators, e.g., 2,5-bis(tert-butylperoxy)-2,5-dimethylhexane, tert-butyl hydroperoxide, and dicumyl peroxide, was also studied. (70-63-7 2,5-Bis(tert-butylperoxy)-2,5-dimethylhexane)(75-91-2 tert-Butyl hydroperoxide)(80-43-3 Dicumyl peroxide) The dechlorination mechanism is probably the same as that of the photosensitized dechlorination. The peroxide-2-propanol systems are applicable to the dechlorination of polychlorinated terphenyls.
 RN - 110-05-4; 67-63-0; 92-52-4; 75-65-0; 67-64-1; 75-63-7; 75-91-2; 80-43-3; 2212-81-9; 7447-40-7; 109-13-7; 2372-21-6
 EH - 7612
- E-6 * SI - CA/087/0581970
 AU - Hamer H ; Batzer OF
 AD - USA
 TI - Organic peroxides as slime settling agents
 SO - U.S. PATENT NO. 4017392 04/12/77 (International Minerals and Chemical Corp.)
 AB - CSAC COPYRIGHT: CHEM ABS A process for settling finely divided waste slime solids from phosphate ore processing comprises adding .gtoreq.1 org. peroxide with mol. wt. .ltoreq.225 in the amt. 10 lb/ton suspended solids. For example, 1 hr after the addn. of 0.32 mL di-tert-butyl peroxide to 100 mL phosphate slime contg. 4.51% suspended solids, the amt. of clear supernatant water was 5 times that of a control. (110-05-4 Di-tert-butyl peroxide)
 RN - 110-05-4; 75-91-2; 79-21-0; 80-15-9; 124-43-6; 3006-82-4
 EH - 7602

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File

DI-tert-BUTYL PEROXIDE

By

**Clement Associates, Inc.
1010 Wisconsin Avenue, NW
Washington, DC 20007**

July 20, 1978

Contract No. EQ8AC013

Prepared for

**TSCA Interagency Testing Committee
Washington, DC**

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DI-tert-BUTYL PEROXIDE

OVERVIEW

Di-tert-butyl peroxide is a colorless liquid that is insoluble in water and soluble in organic solvents. It is used as a chemical intermediate, a polymerization catalyst, and an ignition accelerator for diesel fuel.

Approximately 3 million pounds of di-tert-butyl peroxide were produced in the United States in 1976. No information on occupational exposure was found in the sources searched.

Because of its appreciable vapor pressure, di-tert-butyl peroxide is likely to enter the atmosphere if released. It is a highly reactive compound that forms free radicals and can act as a strong oxidizing agent. Its major degradation products, by reduction and slow hydrolysis, are tert-butyl alcohol and tert-butyl hydroperoxide.

Di-tert-butyl peroxide is considered relatively harmless or slightly toxic. By all routes of exposure, it is far less toxic than its monomeric hydroperoxide, tert-butyl hydroperoxide.

No neoplastic effects were attributed to di-tert-butyl peroxide in a carcinogenicity assay in which the compound was applied to the skin of female Swiss mice. Results of mutation assays in Neurospora and Pneumococcus were also negative.

DI-tert-BUTYL PEROXIDE

III. BIOLOGICAL INFORMATION

A. Effects on Humans

An abstract of a Russian study by Dautov (1977) reported that workers engaged for unspecified times in the production of organic peroxides (including di-tert-butyl peroxide) showed signs of grippe, angina, acute respiratory disease, and pneumonia.

Comment: These effects should not be attributed to di-tert-butyl peroxide alone because, as reported in the abstract, methyl ethyl ketone, benzyl chloride, ammonia, tert-butyl alcohol, hydrogen peroxide, and hydrochloric acid also polluted the atmosphere.

B. Tests on Laboratory Organisms

1. Metabolism

No information was found in the sources searched.

2. Toxic Effects

a. Acute Toxicity

The acute toxicity of di-tert-butyl peroxide, as reported in the NIOSH RTECS data base (1978) and by Floyd and Stokinger (1958), is given in Table III-1.

Floyd and Stokinger (1958) considered di-tert-butyl peroxide relatively harmless or only slightly toxic, far less toxic than its monomeric hydroperoxide, tert-butyl hydroperoxide, by all routes of exposure.

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TABLE III-1
ACUTE TOXICITY OF DI-tert-BUTYL PEROXIDE

Parameter	Dosage	Animal	Route
LD50 ^{1,2}	3,210 mg/kg	Rat	Intraperitoneal
TDLo ¹	580 mg/kg	Mouse	-
LD50 ²	>25,000 mg/kg	Rat	Oral
LC50 ²	>4,103 ppm for 4 hr	"	Inhalation
LC50 ²	>4,103 ppm for 4 hr	Mouse	"

¹Toxicity data from NIOSH 1978

²Toxicity data from Floyd and Stokinger 1958

Adult male Wistar rats given a single intraperitoneal injection of di-tert-butyl peroxide at 2,000-5,000 mg/kg showed porphyrin deposition in the nostrils and shivering (Floyd and Stokinger 1958). When exposed by inhalation to di-tert-butyl peroxide at 4,103 ppm, six rats all developed head and neck tremors in 10 minutes and, at the end of a 4-hour exposure, remained prostrate, with the tremors having virtually disappeared. Mice exposed by inhalation were less affected than rats, exhibiting only excitability and irregular labored breathing.

Floyd and Stokinger (1958) also reported that di-tert-butyl peroxide was nonirritating to the skin and eyes of rabbits.

b. Carcinogenicity

Safficetti and Shubik (1963) observed no tumors after applying a 0.5% solution of di-tert-butyl peroxide in acetone to the skin

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in the interscapular region of 20 female Swiss mice twice a week for 81 weeks. They also conducted a two-stage skin carcinogenicity study in which they applied a 0.5% solution of di-tert-butyl peroxide in acetone to the skin of 20 female Swiss mice twice a week for 3 weeks and beginning 1 week later applied a 5% solution of croton oil in mineral oil twice a week for 80 weeks. The authors reported that one papilloma developed and regressed in an exposed mouse during the 80-week study, as did one in a mouse in a control group of 240 female mice.

c. Mutagenicity and Cell Transformation

According to Jensen et al. (1951), findings in Neurospora back-mutation tests indicated that di-tert-butyl peroxide was nonmutagenic. They gave no experimental details.

Latarjet et al. (1958) added di-tert-butyl peroxide to DNA extracted from streptomycin-resistant Pneumococcus bacteria. They reported that it did not inactivate the DNA's ability to transform sensitive bacteria into resistant ones.

d. Teratogenicity, Embryotoxicity, and Fetotoxicity

No information was found in the sources searched.

e. Other Toxicity

Floyd and Stokinger (1958) reported that a dosage of 1/5 the intraperitoneal LD50 of di-tert-butyl peroxide administered three times a week for 7 weeks caused no deaths in rats. The same regimen at 1/5 the oral LD50, however, was fatal to two out of five rats within 3 weeks. The authors also reported that the

albumin/globulin ratio in rabbits increased over a 2-week period after 0.1 ml of the compound had been applied three times to their skin.

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