

## MATERIAL SAFETY DATA SHEET

DATE PRINTED: 9/12/1997

PAGE 6  
MSDS NO. 15-052531

KORTACID 0899

## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

VAPOR PRESSURE (mm Hg)  
LT 1 @ 20 CVAPOR DENSITY (Air = 1.0)  
N/DEVAPORATION RATE  
LT 1 Butylacetate = 1VOLATILE X  
AP 1 % by weightBOILING POINT  
462.20 F 239.00 C  
at 760 mmHg (minimum)ODOR THRESHOLD (ppm)  
N/DSPECIFIC GRAVITY  
EQ .909 @ 20 CBULK DENSITY  
N/DSOLUBILITY IN WATER  
Practically insolubleSOLUBILITY IN OTHER SOLVENTS  
Soluble in most organic solv.COEFFICIENT OF OIL/WATER  
N/DPOUR POINT  
68.00 F 20.00 C  
ApproximatelyMELTING POINT  
60.80 F 16.00 C  
ApproximatelypH FACTOR  
AP 3-4CLOUD POINT  
N/D F N/D CFLASH POINT  
269.60 F 132.00 CFLASH METHOD  
Pansky-Martens Closed CupUPPER EXPLOSION LIMIT  
N/DLOWER EXPLOSION LIMIT  
N/DAUTO IGNITION TEMPERATURE  
572.00 F 300.00 C  
Greater thanOther  
Viscosity @ 20 C = 5.8 mPa.s

## SECTION 10. STABILITY AND REACTIVITY

**Stability**

This product is stable at ambient temperatures and atmospheric pressures. It is not self-reactive and has a shelf life of greater than one year under sealed conditions. It is not sensitive to physical impact or static discharge.

**Incompatibilities**

This product is incompatible with strong bases and strong oxidizers.

**Polymerization**

Hazardous polymerization is not expected to occur.

**Decomposition**

Under non-oxidizing conditions and when subjected to temperatures in excess of 300 C, this material will decompose into hydrocarbons, carbon monoxide and carbon dioxide.

**Conditions to Avoid**

Contact with strong bases and strong oxidizers and prolonged storage at elevated temperatures should be avoided.

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Akzo Nobel Chemicals Inc.

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SECTION 11. TOXICOLOGICAL INFORMATION  
-----**Toxicological - Inhalation**

Inhalation toxicity data are not available for this product or its components. Because of its low vapor pressure, significant amounts of airborne vapors are not expected at normal room temperatures. However, use at elevated temperatures may generate vapors which are irritating to the respiratory tract.

**Inhalation Chronic Exposure**

Chronic inhalation exposure effects of this product are not known. However, it may cause irritation of the respiratory tract.

**Toxicological - Dermal**

The acute dermal LD50 (rabbit) is > 2000 mg/kg. This material is considered severely irritating and corrosive to skin.

**Skin Contact - CHRONIC**

Chronic dermal exposure effects for this product are not known. However, prolonged or repeated contact can cause severe skin irritation or burns with redness, swelling and blistering.

**Toxicological - Eye**

While this product has not been tested, it is expected to be severely irritating and corrosive to eyes based on animal tests with similar products.

**Toxicological - Ingestion**

The acute oral LD50 (rat) for this material is > 2000 mg/kg. This material is considered severely irritating and corrosive to tissue. Ingestion is expected to cause severe irritation or chemical burns of the mouth, throat, esophagus and any parts of the gastrointestinal system that come in contact with this material.

**Ingestion - CHRONIC**

Chronic ingestion effects of this product are not known. However, ingestion can result in severe irritation or burns of the mouth, throat, esophagus and stomach.

**CARCINOGENICITY/MUTAGENICITY**

The carcinogenic/mutagenic properties of this material are not known.

Neither this material nor its components is classified as a carcinogen or suspect carcinogen by IARC, NTP, OSHA, or ACGIH.

**REPRODUCTIVE EFFECTS**

The reproductive toxicity of this product is not known.

**NEUROTOXICITY**

The neurotoxic effects of this product are not known.

**Other Toxicological Effects**

No other toxic effects for this product are known.

**Target Organs**

Overexposure to this product may affect the skin and eyes.

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SECTION 12. ECOLOGICAL INFORMATION

ECOTOXICOLOGICAL INFORMATION

The ecological toxicity of this product is not known.

DISTRIBUTION

Other ecological information on this product is not known.

CHEMICAL FATE

This product is readily biodegradable.

SECTION 13. DISPOSAL CONSIDERATIONS

Waste Disposal

Material that cannot be used or chemically reprocessed and empty containers, except those designed for multiple use (returnable), should be disposed of in accordance with all applicable regulations. Product containers designed for single use should be thoroughly emptied before disposal. Multiple use containers should be thoroughly emptied before returning to the shipping point.

NOTE] State and local regulations may be more stringent than federal.

This product, if unused, does not meet the RCRA criteria for being identified as a hazardous waste by characteristics. Generators of waste material are required to evaluate all waste for compliance with RCRA and any local disposal procedures and regulations.

CONTAINER DISPOSAL

Containers should be cleaned of residual product before disposal. Do not contaminate public waters with waste or rinsate. Empty containers should be disposed of in accordance with all applicable laws and regulations.

SECTION 14. TRANSPORT INFORMATION

SHIPPING DESCRIPTION

CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S.

(Fatty Acids)

UN 3245

Hazard Class: 8; Packing Group: III

Emergency Response Guide No. 153

REQUIRED LABELS

Corrosive

ENVIRON. HAZARDOUS SUBSTANCE

This product does not contain an environmentally hazardous substance per 49 CFR 172.101, Appendix B.

SECTION 15. REGULATORY INFORMATION

Component Octanoic acid is subject to the following

Environmental List

DSL	Domestic Substance List-Canada
TSCA	Toxic Subst. Cont. Act -listed

Akzo Nobel Chemicals Inc.

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SECTION 15. REGULATORY INFORMATION  
(CONTINUED)

Component Hexanoic acid is subject to the following

## Environmental List

DSL	Domestic Substance List-Canada
MA. LIST	Massachusetts Substance List
NJ R-T-K	New Jersey R-T-K Hazard. Sub.
PA. LIST	Penn. Hazardous Substance List
TSCA	Toxic Subst. Cont. Act -listed

Component Decanoic acid is subject to the following

## Environmental List

DSL	Domestic Substance List-Canada
TSCA	Toxic Subst. Cont. Act -listed

## OTHER REGULATORY INFORMATION

No other regulatory information is available on this product.

WHMIS HAZARD CLASS  
D-2B, EHAZARD RATING SOURCE  
HMISHEALTH  
3REACTIVITY  
0FLAMMABILITY  
1

OTHER

## SECTION 16. OTHER INFORMATION

## OTHER INFORMATION

KORTACID is a registered trademark of Akzo Nobel Chemicals Inc.

CREATED BY  
PRODUCT SAFETY 914/674-5000

## KEY TO ABBREVIATIONS:

EQ=Equal  
AP=ApproximatelyLT=Less Than  
TR=TraceGT=Greater Than  
ND=No Data available

All information concerning this product and/or suggestions for handling and use contained herein are offered in good faith and are believed to be reliable. Akzo Nobel Chemicals Inc. assumes no liability as to the accuracy or sufficiency of this information and/or suggestions, as to the product's merchantability or fitness for any particular purpose, or that any suggestion we will not involve any patent. Nothing contained herein shall be construed as granting or extending any license under any patent. Paper and literature for itself, by preliminary tests or otherwise, the suitability of this product for all purposes. The information contained herein supersedes all previously issued literature on the subject matter covered.

RETURN TO MENU

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**PEROXYOCTANOIC ACID**  
**MATERIAL SAFETY DATA SHEET**

Ecolab Inc.  
Ecolab Center, St. Paul MN 55102  
Product Information: 1-651-293-4255

Issue Date: October 22, 1999

1.0 IDENTIFICATION /

- 1.1 Product Name: PEROXYOCTANOIC ACID
- 1.2 Product Type: Aliphatic Peroxide
- 1.3 Hazard Rating: Health: 2 Fire: 0 Reactivity: 1

Substances Subject to SARA 313 Reporting Are Indicated by "#"

2.0 HAZARDOUS COMPONENTS /

- |                          | CAS No.    | (mg/m3) | PEL | TWA |
|--------------------------|------------|---------|-----|-----|
| 2.1 Peroxyoctanoic acid* | 33734-57-5 |         | No  | No  |
- \*this material exists only in an equilibrium state with octanoic acid and hydrogen peroxide. It is not isolated in a pure form. This MSDS presents information based on the best scientific evidence available, not on actual product testing.

PEL = OSHA 8 hour average in air

TWA = ACGIH 8 hour average in air

3.0 PHYSICAL DATA /

- 3.1 Appearance: Waxy white solid
- 3.2 Solubility in Water: Slightly soluble
- 3.3 pH: 3 - 4 (estimated pH of aqueous solution)

4.0 FIRE AND EXPLOSION DATA /

- 4.1 Special Fire Hazards: Decomposition of product releases oxygen which may intensify fire. See Section 5. Oxidizer.
- 4.2 Fire Fighting Methods: Flood fire-exposed containers to cool them.

5.0 REACTIVITY DATA /

- 5.1 Stability: Heat or contaminants can cause decomposition of product. Store in a cool area.
- 5.2 Conditions to Avoid: Avoid excessive heat, organic contaminants of any kind, contact with iron or copper.

6.0 SPILL OR LEAK PROCEDURES / WEAR PROPER PROTECTIVE EQUIPMENT

- 6.1 Cleanup: Sweep up, using inert material (earth, sand, etc.). Rinse area with water.
- 6.2 Waste Disposal: Consult state/local authority for limits on chemical waste disposal.

090417

Product: PEROXYOCTANOIC ACID  
Ecolab Inc.

MEDICAL EMERGENCY ONLY, 24 HOUR SERVICE: 1-800-328-0026

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7.0 HEALTH HAZARD DATA /

WARNING

7.1 Effects of Overexposure to Concentrate:

Eyes: Causes severe irritation or eye damage.

Skin: Causes severe irritation or skin damage.

If Swallowed: May be harmful or fatal if swallowed.

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8.0 FIRST AID /

8.1 Eyes: Flush at once with cool running water. Remove contact lenses and continue flushing for 15 minutes, holding eyelids apart so as to rinse entire eye. CALL A PHYSICIAN IMMEDIATELY.

8.2 Skin: Immediately wash with plenty of soap and water. Get medical attention. Remove and wash contaminated clothing before reuse.

8.3 If Swallowed: Rinse mouth at once; then drink 1 or 2 large glasses of water. DO NOT induce vomiting. NEVER give anything by mouth to an unconscious person.

IMMEDIATELY CALL THE MEDICAL EMERGENCY NUMBER, 1-800-328-0026,  
A POISON CONTROL CENTER, OR A PHYSICIAN

Note to Physician: Probable mucosal damage may contraindicate the use of gastric lavage.

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9.0 PROTECTIVE MEASURES /

9.1 FOR CONCENTRATE:

Eyes: Wear chemical splash goggles.

Skin: Wear any industrial rubber gloves, synthetic apron, other protective equipment as necessary to prevent skin contact. Wash well after handling product.

Respiratory: Avoid breathing mists or vapors of this product.

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10.0 ADDITIONAL INFORMATION /

10.1 Purpose of 10/24/1999 issue: First issue. This MSDS provides information on a non-isolated component in a finished product. This document prepared for product evaluation by regulatory authorities.

KEEP OUT OF REACH OF CHILDREN

The above information is believed to be correct with respect to the formula used to manufacture the product. As data, standards, and regulations change, and conditions of use and handling are beyond our control, NO WARRANTY, EXPRESS OR IMPLIED, IS MADE AS TO THE COMPLETENESS OR CONTINUING ACCURACY OF THIS INFORMATION.

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**HEDP**  
**MATERIAL SAFETY DATA SHEET**

Monsanto MSDS Name: DEQUEST® 2010 DEFLOCCULANT AND SEQUESTERANT (002909214)



# Monsanto

## Material Safety Data Sheet

**PRODUCT NAME:** DEQUEST® 2010 DEFLOCCULANT AND SEQUESTERANT

**MONSANTO COMPANY,** 800 N. LINDBERGH BLVD., ST. LOUIS, MO 63167

**FOR CHEMICAL EMERGENCY, SPILL LEAK, FIRE, EXPOSURE, OR ACCIDENT**

Call CHEMTREC - Day or Night - 1-800-424-9300 Toll free in the continental U.S., Hawaii, Puerto Rico, Canada, Alaska, or Virgin Islands. For calls originating elsewhere: 703-527-3887 (collect calls accepted)

For additional non-emergency information, call: 314-694-6661

### PRODUCT IDENTIFICATION

<b>Synonym(s):</b>	HEDP; 1-Hydroxyethylidene-1,1-diphosphonic acid, etidronic acid
<b>Chemical Name:</b>	Phosphonic acid, (1-hydroxyethylidene)bis-
<b>Chemical Formula:</b>	C(OH)(CH <sub>3</sub> )(PO <sub>3</sub> H <sub>2</sub> ) <sub>2</sub>
<b>Chemical Family:</b>	Phosphonates
<b>CAS No.:</b>	2809-21-4
<b>TSCA Inventory:</b>	Phosphonic acid, (1-hydroxyethylidene)bis- appears on the inventory of Chemical Substances published by the U.S. Environmental Protection Agency (EPA) under authority of the Toxic Substances Control Act (TSCA).
<b>DOT Proper Shipping Name:</b>	Corrosive Liquid, acidic, organic, N.O.S. (contains phosphonic acid)
<b>DOT Hazard Class/LD. No./</b>	
<b>Packing Group:</b>	8/UN3265/PG III
<b>DOT Label:</b>	Corrosive
<b>U.S. Surface Freight Classification:</b>	Washing Compound, N.O.I.B.N., Liquid
<b>Reportable Quantity (RQ) Under</b>	
<b>U.S. EPA CERCLA Regulations:</b>	Not Applicable

#### SARA Hazard Notification

Hazardous Categories Under Criteria  
of SARA Title III Rules

Monsanto MSDS Name: DEQUEST® 2010 DEFLOCCULANT AND SEQUESTRANT (002809214)

(40 CFR Part 370):

Immediate

Section 313 Toxic Chemical(s): Not Applicable

Hazardous Chemical(s) Under OSHA Hazard Communication Standard:

This product contains, as components, the substances listed below which are identified as hazardous chemicals under the criteria of the OSHA Hazard Communication Standard (29 CFR 1910.1200):

1-Hydroxyethylidene-1,1-diphosphonic acid, CAS Reg. No. 2309-21-4

Phosphorous Acid, CAS Reg. No. 10294-56-1

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## WARNING STATEMENTS

**DANGER!**

**CAUSES EYE BURNS**

**CORROSIVE TO MILD STEEL**

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## PRECAUTIONARY MEASURES

Do not get in eyes, on skin or clothing.

Avoid breathing vapor or mist.

Keep container closed.

Use with adequate ventilation.

Wash thoroughly after handling.

Emptied container retains vapor and product residue. Observe all labeled safe-guards until container is cleaned, reconditioned or destroyed.

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## EMERGENCY AND FIRST AID PROCEDURES

**FIRST AID: IF IN EYES,** immediately flush with plenty of water for at least 15 minutes. Get medical attention. Remove material from skin and clothing.

**IN CASE OF: SPILL OR LEAK,** contain spills and leaks to prevent discharge to the environment.

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## OCCUPATIONAL CONTROL PROCEDURES

**Eye Protection:** Where there is potential for eye contact, wear chemical goggles and have eye flushing equipment immediately available.

**Skin Protection:** Although Dequest 2010 does not present a significant skin concern, skin contamination should be minimized by following good industrial practice. Wearing of protective gloves is recommended. Wash hands and contaminated skin after handling.

**Respiratory Protection:** Avoid breathing vapor or mist. Use NIOSH/MSHA approved respiratory protection equipment (full facepiece recommended) when airborne exposure is excessive. If used, full facepiece replaces need for chemical goggles. Consult respirator manufacturer to determine appropriate type equipment for given application. The respirator use limitations specified by NIOSH/MSHA or the manufacturer must be observed. Respiratory protection programs must be in compliance with 29 CFR 1910.134.

**Ventilation:** Provide ventilation to minimize exposure. Use local mechanical exhaust ventilation at sources of air contamination such as open process equipment.

Monsanto MSDS Name: DEQUEST® 2010 DEFLOCCULANT AND SEQUESTANT (002809214)

**Airborne Exposure Limits:**

**DEQUEST 2010**

OSHA PEL: None established  
ACGIH TLV: None established

**Components:**

1-Hydroxyethylidene-1,1-diphosphonic acid (typically 60% by weight of product)

OSHA PEL: None established  
ACGIH TLV: None established

Phosphorous Acid (typically 3% by weight of product)

OSHA PEL: None established  
ACGIH TLV: None established

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**FIRE PROTECTION INFORMATION**

Although this material does not meet the parameters for flammability, it will burn in the presence of a strong ignition source after the water is removed.

**Extinguishing Media:** Water spray, dry chemical, CO<sub>2</sub>, or other Class B extinguishing agent.

**Special Firefighting Procedures:** When DEQUEST 2010 is involved in a fire, firefighters or others should wear full protective clothing and self-contained breathing apparatus if exposed to vapors or products of combustion. All fire fighting equipment, including protective clothing and self-contained breathing apparatus, needs to be decontaminated after use.

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**REACTIVITY DATA**

**Materials to Avoid:** Avoid contact with concentrated caustic. Contact will result in the evolution of heat. Also, avoid contact with strong oxidizing agents.

**Hazardous Decomposition Products:** Phosphines may form after all the water has been removed. CO, CO<sub>2</sub>, and oxides of phosphorus may also be formed.

**Hazardous Polymerization:** Does not occur.

**Incompatibility:** Severely corrosive to steel based on DOT, 49 CFR criteria.

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**HEALTH EFFECTS SUMMARY**

The following information summarizes human experience and results of scientific investigations reviewed by health professionals for hazard evaluation of DEQUEST 2010 Deflocculant and Sequestant and development of Precautionary Statements and Occupational Control Procedures recommended in this document.

**Effects of Exposure**

Skin contact is expected to be the primary route of occupational exposure to DEQUEST 2010 Deflocculant & Sequestant. Though occupational exposure to this material has not been reported to cause significant adverse health effects, DEQUEST 2010 deflocculant is considered, on the basis of acute animal tests, to be corrosive to the eyes.

Monsanto MSDS Name: DEQUEST® 2010 DEFLOCCULANT AND SEQUESTRANT (002809214)

### Toxicological Data

Data from Monsanto studies indicate the following:

Oral -	Slightly Toxic	(Rat LD50: 2400 mg/kg)
Dermal -	Practically Nontoxic	(Rabbit LD50: >7940 mg/kg)
Eye Irritation -	Corrosive	
Skin Irritation -	Nonirritating	(Rabbit, 24 hr., 0.0/8.0)

Following repeated exposures (90 days) to DEQUEST 2010 deflocculant (usually as the sodium salt) in their feed, rats showed minor changes in one study and no adverse effects in another; dogs dosed orally (30 days) also showed only minor changes in one study but not in another. Rats given this material in the diet for 2 years had only minor changes to the adrenal gland which may not have been related to treatment. Dogs given the test material in the diet for 2 years developed an anemia which corrected itself during the study. However dogs given the test material by injection under the skin or by direct oral dosing (capsules) developed severe effects on the bone, with rib and pelvic fractures reported in many of the animals.

No birth defects were noted in rats or rabbits given DEQUEST 2010 deflocculant (as the sodium salt) orally during pregnancy. No effects were seen on the ability of male and female rats to reproduce when given DEQUEST 2010 deflocculant (as the sodium salt) in their diet for 2 successive generations.

DEQUEST 2010 deflocculant produced no genetic changes in standard *in vitro* assays using bacterial and mammalian cells.

### Components

Data from laboratory studies conducted by Monsanto and from the scientific literature on phosphoric acid, a component of DEQUEST 2010 Deflocculant which have been identified under the criteria of the OSHA Hazards Communication Standard (29 CFR 19190.1200):

#### Phosphorous Acid

Phosphorous acid is considered to be slightly toxic following oral administration to rats and dermal administration to rabbits. It is corrosive to eyes and skin and, thus, may contribute to the irritation potential of DEQUEST 2010 deflocculant. Phosphorus acid produced no genetic changes in standard tests using bacteria.

### Additional Information

Hydroxyethylidene-1,1-diphosphonic acid (HEDP), the active acid in DEQUEST 2010 Deflocculant, has established therapeutic application in treatment of certain bone related diseases due to its ability to alter the development of the bone mineral matrix. Many clinical observations on the use of HEDP in bone disease and skeletal imaging have been published. Additional publications extensively discuss the effects of HEDP on bone mineralization and on calcium and phosphate metabolism in man and laboratory animals. For additional toxicity information relative to these uses, please refer to the appropriate scientific literature.

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### PHYSICAL DATA

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Appearance:	Clear solution, yellow color
Odor:	Characteristic odor
Freezing Point:	0C (<32F) -22_C (-13_F)

Monsanto MSDS Name: DEQUEST® 2010 DEFLOCCULANT AND SEQUESTERANT (002809214)

Specific Gravity @ 20C/15C: 1.45  
 Viscosity (centistokes) @ 20C: 46.01  
                                   @ 40C: 20.20  
                                   @ 60C: 10.27  
                                   @ 90\_C: 4.96

pH (1% solution @ 25C): <2

Solubility in Water: Capable of being mixed (miscible) in all proportions

NOTE: These physical data are typical values based on material tested by may vary from sample to sample. Typical values should not be construed as a guaranteed analysis of any specific lot or as specification for the product.

### SPILL, LEAK, & DISPOSAL INFORMATION

**Emergency Spill and Leak Information:** When handling spills and leaks, follow good industrial hygiene and safety practices as outlined in the Precautionary Measures and Emergency and First Aid Procedures section of this document. Contain spills and leaks to prevent discharge to the environment. Absorb spillage with clay, sawdust or other absorbent material. Place all spilled material, contaminated sorbent materials, contaminated dirt, and other contaminated material in drums. If possible, it is also acceptable to contain spilled material and recover it as a liquid prior to disposal.

Keep concentrated product out of sewers, watersheds and water systems.

**Disposal Information:** Dispose of in accordance with all applicable local, state and federal regulations.

As currently defined in the federal Resource Conservation & Recovery Act (RCRA), DEQUEST 2000 deflocculant and sequesterant, when discarded, is a hazardous waste exhibiting the characteristic of corrosivity (D-002). See 40 CFR 261.22. Its disposal, therefore, is regulated by federal RCRA regulations. Consult your attorney or appropriate regulatory officials for information regarding additional state and local waste disposal requirements. Disposal by incineration is recommended.

### ENVIRONMENTAL EFFECTS

#### Environmental Toxicity Information:

	<u>96-hr</u>	<u>14-day</u>
<u>Algae* EC50</u>	3 mg/L	39 mg/L
<u>Invertebrates</u>		
Daphnia magna 48-hr EC50, 527 mg/L:		Practically NonToxic
Midge Larvae 48-hr LC50, 8,910 mg/L:		Practically NonToxic
Grass Shrimp 96-hr LC50, 1,770 mg/L:		Practically NonToxic
Oyster Shell Deposition 96-hr EC50, 89 mg/L:		Slightly Toxic
<u>Fish</u>		
Bluegill Sunfish 96-hr LC50, 868 mg/L:		Practically NonToxic
Rainbow Trout 96-hr LC50, 368 mg/L:		Practically NonToxic
Channel Catfish 96-hr LC50, 695 mg/L:		Practically NonToxic
Sheepshead Minnow 96-hr LC50, 2,180 mg/L:		Practically NonToxic
Rainbow Trout 14-day LC50, 180 mg/L:		
<u>Birds</u>		
Mallard Duck Oral LD50, >2,510 mg/kg:		Practically NonToxic

Monsanto MSDS Name: DEQUEST® 2010 DEFLOCCULANT AND SEQUESTANT (002809214)

Bobwhite Quail Oral LD50, >2,510 mg/kg: Practically Non Toxic

*Daphnia magna* were exposed to DEQUEST 2010 concentrations ranging from 3.37 to 400 mg/L for 28 days. Reductions in adult *Daphnia* survival and reproduction were observed at concentrations above 25 mg/L. The maximum acceptable toxicant concentration was greater than 12.5 mg/L and less than 25 mg/L.

Carp were continuously exposed to radiolabeled active acid of DEQUEST 2010 at nominal concentrations of 0.058 and 0.55 mg/L for 49 days, after which remaining fish were transferred to DEQUEST-free water for 14 days. Tissue residue analysis determined that radiolabeled active acid of DEQUEST 2010 did not bioconcentrate in the edible tissues. Radiolabeled residues did accumulate in the non-edible tissues (viscera including ingesta and fecal material). Elimination of the residues from the non-edible tissues of the carp was rapid and extensive after transfer to DEQUEST-free water.

When evaluated in a microbial biodegradation assay, DEQUEST 2010 biodegradation to CO<sub>2</sub> was classified as slow to intermediate.

\* Algae growth inhibition due to the ability of DEQUEST to complex nutrients, not toxicity per se.

NOTE: All values are "mg active acid/liter".

For additional information on this product refer to Monsanto Product Bulletin on DEQUEST 2010 deflocculant and sequestant.

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DEQUEST® is a registered trademark of Monsanto Company

DATE: 8/27/96

SUPERSEDES: 11/19/93

MSDS NUMBER 002809214

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Although the information and recommendations set forth herein (hereinafter "information") are presented in good faith and believed to be correct as of the date hereof, Monsanto Company makes no representations as to the completeness or accuracy thereof. Information is supplied upon the condition that the persons receiving same will make their own determination as to its suitability for their purposes prior to use. In no event will Monsanto Company be responsible for damages of any nature whatsoever resulting from the use of or reliance upon information. NO REPRESENTATIONS OR WARRANTIES, EITHER EXPRESS OR IMPLIED, OF MERCHANTABILITY, FITNESS FOR A PARTICULAR PURPOSE OR OF ANY OTHER NATURE ARE MADE HEREUNDER WITH RESPECT TO INFORMATION OR THE PRODUCT TO WHICH INFORMATION REFERS.

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RETURN TO MENU

MSDS Briquest ADPA-60A

# MATERIAL SAFETY DATA SHEET

**ALBRIGHT  
& WILSON**  
Americas

Date-Issued: 01/29/1996  
MSDS Ref. No: PSMDS-211  
Date-Revised: 08/22/1997  
Revision No: 1  
Briquest ADPA-60A

## 1. CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

PRODUCT NAME: Briquest ADPA-60A  
GENERAL USE: Cleaning Agent  
PRODUCT CODE: 211  
PRODUCT FORMULATION NAME: 1-Hydroxyethane-1,1-Diphosphonic Acid.  
CHEMICAL FAMILY: Organic Phosphonates  
GENERIC NAME: HEDP

### MANUFACTURER

Albright & Wilson Americas Inc.  
Specialty Chemicals Division  
P.O. Box 4439  
Glen Allen, VA 23058-4439  
Contact: Product Stewardship Department  
Product Stewardship: (304) 968-6496  
Transportation: (304) 968-6418

### 24 HR. EMERGENCY TELEPHONE NUMBERS

CHEMTREC (800) 424-9300  
Canutec (613) 996-6666  
Emergency Phone (303) 554-1229

COMMENTS: To the best of our knowledge, this Material Safety Data Sheet conforms to the requirements of US OSHA 29 CFR 1910.1200, 91/155/EEC and Canadian Hazardous Products Act.

## 2. COMPOSITION/INFORMATION ON INGREDIENTS

Chemical Name	Wt. %	CAS Registry #	EINECS #
Phosphonic acid, (1-hydroxyethylidene)bis-	~60	2309-21-4	220-552-8

### EEC LABEL SYMBOL AND CLASSIFICATION



R 41: Risk of serious danger to eyes.  
R 38: Irritating to skin.

EEC Corrosive - "C"

### COMMENTS:

MSDS Briquest ADPA-60A

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Product composition ranges shown are typical values for health, safety and environmental use and are not intended as specifications.

### 3. HAZARDS IDENTIFICATION

#### EMERGENCY OVERVIEW

**PHYSICAL APPEARANCE:** Clear, colorless aqueous solution with slight characteristic odor.

**IMMEDIATE CONCERNS:** DANGER! Causes eye burns and skin irritation.

#### POTENTIAL HEALTH EFFECTS

**EYES:** Will cause corrosive effects (burns or irreversible damage) to the eyes.

**SKIN:** Expected to cause significant irritation to the skin.

**INGESTION:** Expected to cause significant irritation to the digestive tract.

**INHALATION:** Expected to cause significant irritation to the lungs, upper respiratory tract, and nose.

#### SIGNS AND SYMPTOMS OF OVEREXPOSURE

**EYES:** Severe burning of the eyes.

**SKIN:** Redness and possible burning of the skin.

**INGESTION:** Possible nausea and/or vomiting.

**INHALATION:** Coughing, burning, tightness of chest and/or shortness of breath.

#### ACUTE TOXICITY:

Not expected to cause significant adverse effects if absorbed through the skin.

Not expected to cause significant adverse effects if ingested.

No test data is available for acute inhalation toxicity.

#### CARCINOGENICITY:

Not Listed by NTP  
Not listed by IARC  
Not listed by OSHA

#### MUTAGENICITY:

Not Available

#### REPRODUCTIVE TOXICITY

**REPRODUCTIVE EFFECTS:** Not Available

**TERATOGENIC EFFECTS:** Not Available

**MEDICAL CONDITIONS AGGRAVATED:** Possibly skin diseases or anemia.

**TARGET ORGAN STATEMENT:** Contains material which may cause blood, bone, gastrointestinal tract, and respiratory tract effects based on animal data.

MSDS Briquest ADPA-60A

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**SENSITIZATION:** Not Available**COMMENTS:** For detailed toxicological information see Section 11.

#### 4. FIRST AID MEASURES

**EYES:** Immediately flush eyes with plenty of water for two to three minutes. Remove any contact lenses and continue flushing for 15 minutes. Get immediate medical attention.**SKIN:** Remove contaminated clothing including shoes and immediately wash affected area with plenty of soap and water. Seek immediate medical attention. Wash contaminated clothing and shoes before reuse.**INGESTION:** Wash out mouth with water and keep at rest. Seek immediate medical attention.**INHALATION:** Remove from further exposure. Keep warm and at rest. If cough or other symptoms develop, seek medical attention.

#### 5. FIRE FIGHTING MEASURES

**FLASHPOINT AND METHOD:** Not Available**FLAMMABLE LIMITS:** Not Available**AUTOIGNITION TEMPERATURE:** Not Available**FLAMMABLE CLASS:** Nonflammable**FLAME PROPAGATION OR BURNING RATE OF SOLIDS:** Not Applicable**GENERAL HAZARD:** Evacuate personnel downwind of fire to avoid inhalation of irritating and/or harmful fumes and smoke.**EXTINGUISHING MEDIA:** Chemical type foam, CO<sub>2</sub> (Carbon Dioxide), Dry Chemical**HAZARDOUS COMBUSTION PRODUCTS:** Oxides of both carbon and phosphorus**FIRE FIGHTING PROCEDURES:** For small containers of organic substances, it should be considered if there will be less damage by allowing the material to burn to exhaustion rather than fighting the fire and risk causing environmental contamination and other problems.**FIRE FIGHTING EQUIPMENT:** Respiratory and eye protection are required for fire fighting personnel. Full protective equipment (Bunker Gear) and self contained breathing apparatus (SCBA) should be used for all indoor fires and any significant outdoor fires. For small outdoor fires, which may easily be extinguished with a portable fire extinguisher, use of a SCBA may not be required.**SENSITIVE TO STATIC DISCHARGE:** Not Available**SENSITIVITY TO IMPACT:** Not Available

#### 6. ACCIDENTAL RELEASE MEASURES

**SMALL SPILL:**

Construct temporary dikes of dirt, sand, or any appropriate readily available material to prevent spreading of the material.

Wearing the appropriate personal protective equipment designated in Section 8, move the leaking container to a containment area or rotate the container so that the opening is above the liquid level.

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Absorb on diatomaceous earth or equivalent inert material. Shovel up and dispose of at an appropriate waste disposal facility according to current applicable laws and regulations, and product characteristics at time of disposal.

**LARGE SPILL:**

Construct temporary dikes of dirt, sand, or any appropriate readily available material to prevent spreading of the material.

Wearing the appropriate personal protective equipment designated in Section 8, close or cap valves and/or block or plug hole in leaking container and transfer to another container.

Contain material as described above and call the local fire or police department for immediate emergency assistance.

**ENVIRONMENTAL PRECAUTIONS**

**WATER SPILL:** Use appropriate containment to avoid runoff or release to sewer or waterways.

**LAND SPILL:** Use appropriate containment to avoid runoff or release to ground.

**GENERAL PROCEDURES:** Remove containers of strong oxidizers and strong bases from release area.

**RELEASE NOTES:** If spill could potentially enter any waterway, including intermittent dry creeks, contact the local authorities. If in the U.S., contact the US COAST GUARD NATIONAL RESPONSE CENTER toll free number 800-424-8302.

In case of accident or road spill notify:  
CHEMTREC in USA at 800-424-9300  
CANUTEC in Canada at 613-996-6666  
CHEMTREC, other countries, at (International code)+1 202 483 7616

**COMMENTS:**

See Section 13 for disposal information and Section 15 for regulatory requirements. Large and small spills may have a broad definition depending on the user's handling system. Therefore, the spill category must be defined at the point of release by technically qualified personnel.

**7. HANDLING AND STORAGE****HANDLING:**

Use appropriate personal protective equipment as specified in Section 8. Handle in a well ventilated area.

Handle and use in a manner consistent with good industrial/manufacturing techniques and practices.

**STORAGE:**

Store in unopened containers under cool and dry conditions.

Do not store with, or close to oxidizers and bases.

**8. EXPOSURE CONTROLS/PERSONAL PROTECTION****EXPOSURE GUIDELINES:**

**OSHA HAZARDOUS COMPONENTS (29 CFR 1910.1200)**

**EXPOSURE LIMITS**  
**OSHA PEL ACGIH TLV Supplier OEL**  
**ppm mg/m<sup>3</sup> ppm mg/m<sup>3</sup> ppm mg/m<sup>3</sup>**

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Phosphonic acid, (1-hydroxyethylidene)bis-

TWA	NL <sup>(1)</sup>	NL	NL	NL	NL
STEL	NL	NL	NL	NL	NL

**OSHA TABLE COMMENTS:**

1. NL = Not Listed

**ENGINEERING CONTROLS:** Good ventilation should be sufficient to control airborne levels of material.**PERSONAL PROTECTIVE EQUIPMENT****EYES AND FACE:** Wear chemical splash goggles and face shield when eye and face contact is possible due to splashing or spraying of material.**SKIN:** Where contact is likely, wear neoprene chemical resistant gloves, a chemical suit, rubber boots, chemical safety goggles and a face shield.**RESPIRATORY:** Always wear NIOSH approved respiratory protective equipment when there may be potential for airborne exposure.**WORK HYGIENIC PRACTICES:** Facilities storing or using this material should be equipped with an eyewash facility and a safety shower.  
Good personal hygiene practices should always be followed.**COMMENTS:** No PEL's, TLV's or OEL's for this product or its ingredients are listed in the current issue of ACGIH's Guide to Occupational Exposure Values nor have they been determined by the manufacturer.**9. PHYSICAL AND CHEMICAL PROPERTIES****PHYSICAL STATE:** Liquid**ODOR:** Slight characteristic**APPEARANCE:** Clear**COLOR:** Colorless**pH:** 1.0 of a 1% solution**VAPOR PRESSURE:** 17 mmHg at 20°C (68°F)**VAPOR DENSITY:** Not Available**BOILING POINT:** >100°C (212°F)**FREEZING POINT:** Not Available**MELTING POINT:** Not Available**SOLUBILITY IN WATER:** Miscible**EVAPORATION RATE:** Not Available**DENSITY:** 1.46 g/ml at 20°C (68°F)**SPECIFIC GRAVITY:** 1.46 @ 20°C/4°C**VISCOSITY:** 64 Centipoise at 20°C (68°F)

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MOLECULAR FORMULA:  $C_2H_3O_7P_2$

MOLECULAR WEIGHT: 206 g/mol

COEFF. OIL/WATER: Not Applicable

## 10. STABILITY AND REACTIVITY

STABLE: YES

HAZARDOUS POLYMERIZATION: NO

CONDITIONS TO AVOID: Heat, Temperatures above 200 °C.

STABILITY: The product is stable under normal ambient conditions of temperature and pressure.

POLYMERIZATION: Will not occur

HAZARDOUS DECOMPOSITION PRODUCTS: Oxides of both phosphorus and carbon, acids of phosphorus and phosphine.

INCOMPATIBLE MATERIALS: Strong Oxidizers  
Strong bases

## 11. TOXICOLOGICAL INFORMATION

### ACUTE

DERMAL LD<sub>50</sub>: Dermal LD50(rabbit) > 10000 mg/kg

ORAL LD<sub>50</sub>: Oral LD50(rat) > 2000 mg/kg

INHALATION LC<sub>50</sub>: Not Available

EYE EFFECTS: This material is corrosive to the eyes.

SKIN EFFECTS: This material is expected to cause significant irritation to the skin.

SENSITIZATION: Not Available

TARGET ORGANS: Eyes

Blood

Skin

Gastrointestinal tract

Respiratory system

Bone/Teeth

### CARCINOGENICITY:

Listed by IARC - No

Listed by NTP - No

Listed by OSHA - No

MUTAGENICITY: Not Available

REPRODUCTIVE EFFECTS: Not Available

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**TERATOGENIC EFFECTS:** Not Available**GENERAL COMMENTS:** Possible skeletal effects; may decrease the affinity of hemoglobin for oxygen. Fetal anomalies have been reported in mice.

## 12. ECOLOGICAL INFORMATION

**ENVIRONMENTAL DATA:** Not expected to cause significant adverse environmental impact if material reaches waterways.**ECOTOXICOLOGICAL INFORMATION:** 96 hr, LC50(rainbow trout) > 368 mg/L  
48hr, EC50 (Daphnia) = 527 mg/L  
LC50(algae)-10-100 mg/l, due to the nutrient chelating ability of phosphonates, these results may not accurately reflect their toxicity.  
Not toxic to aquatic organisms and not suspected of long-term adverse effects in the aquatic environment**DISTRIBUTION:** Not Available

## 13. DISPOSAL CONSIDERATIONS

**DISPOSAL METHOD:** Dispose of waste at an appropriate waste disposal facility according to current applicable laws and regulations.**FOR LARGE SPILLS:** Contain material and call local authorities for emergency assistance. In consultation with the appropriate authorities, determine the disposal method or contact Albright & Wilson Americas.**PRODUCT DISPOSAL:** Dispose of at a supervised incineration facility or an appropriate waste disposal facility according to current applicable laws and regulations and product characteristics at time of disposal.**EMPTY CONTAINER:** Rinse drums with a suitable solvent and steam to remove vapors before disposal or reuse in accordance with applicable regulations.**GENERAL COMMENTS:** Refer to Section 6, Accidental Release Measures for additional information.

## 14. TRANSPORT INFORMATION

### DOT (DEPARTMENT OF TRANSPORTATION)

**PROPER SHIPPING NAME:** Corrosive Liquid, Acidic, Organic N.O.S.**TECHNICAL NAME:** 1 - Hydroxyethane - 1, 1 - Diphosphonic Acid**PRIMARY-HAZARD CLASS/DIVISION:** 8**UN/NA NUMBER:** UN3265**PACKING GROUP:** II**LABEL:** Corrosive**NAERG:** 153

### CANADA TRANSPORT OF DANGEROUS GOODS

**PROPER SHIPPING NAME:** Corrosive Liquid, Acidic, Organic N.O.S.

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TECHNICAL NAME: 1 - Hydroxyethane - 1, 1 - Diphosphonic Acid

PRIMARY HAZARD CLASS/DIVISION: 8

UN/NA NUMBER: UN 3265

PACKING GROUP: II

LABEL: Corrosive

AIR (ICAO/IATA)

PROPER SHIPPING NAME: Corrosive Liquid, Acidic, Organic N.O.S.

TECHNICAL NAME: 1 - Hydroxyethane - 1, 1 - Diphosphonic Acid

PRIMARY HAZARD CLASS/DIVISION: 8

UN/NA NUMBER: UN 3265

PACKING GROUP: II

LABEL: Corrosive

VESSEL (IMO/MDG)

PROPER SHIPPING NAME: Corrosive Liquid, Acidic, Organic N.O.S.

TECHNICAL NAME: 1 - Hydroxyethane - 1, 1 - Diphosphonic Acid

PRIMARY HAZARD CLASS/DIVISION: 8

UN/NA NUMBER: UN 3265

PACKING GROUP: II

LABEL: Corrosive

EUROPEAN TRANSPORTATION:

ADR/RID ITEM NUMBER: 40°C

U.S. CUSTOMS HARMONIZATION NUMBER: 2931.00.90.30

15. REGULATORY INFORMATION

UNITED STATES

DOT LABEL SYMBOL AND HAZARD CLASSIFICATION



DOT Corrosive

SARA TITLE III (SUPERFUND AMENDMENTS AND REAUTHORIZATION ACT)

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311/312 HAZARD CATEGORIES:

FIRE: NO PRESSURE GENERATING: NO REACTIVITY: NO ACUTE: YES CHRONIC: NO

313 REPORTABLE INGREDIENTS: Not Applicable

TITLE III NOTES: Not Applicable

CERCLA (COMPREHENSIVE RESPONSE, COMPENSATION, AND LIABILITY ACT)

CERCLA RQ: Not Applicable

TSCA (TOXIC SUBSTANCE CONTROL ACT)

TSCA REGULATORY: All intentional ingredients are listed on the TSCA Inventory.

NATIONAL RESPONSE CENTER: U.S. Coast Guard National Center telephone # 1-800-424-8802

CANADA

WHMIS HAZARD SYMBOL AND CLASSIFICATION



Corrosive, Class E

WHMIS Corrosive

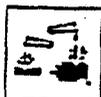
WHMIS (WORKER HAZARDOUS MATERIALS INFORMATION SYSTEM): This product is WHMIS controlled.

CANADA INGREDIENT DISCLOSURE LIST: This product does not contain any known ingredient(s) on the "Ingredient Disclosure List".

CANADIAN ENVIRONMENTAL PROTECTION ACT: All intentional ingredients are listed on the DSL (Domestic Substance List).

EUROPEAN COMMUNITY

EEC LABEL SYMBOL AND CLASSIFICATION



R 41: Risk of serious danger to eyes.

R 38: Irritating to skin.

S 39: Wear eye/face protection.

S 24, S 25: Avoid contact with skin or eyes.

S 26: In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

S 23: After contact with skin, wash immediately with plenty of soap and water.

EEC Corrosive - "C"

EUROPEAN COMMUNITY REGULATORY: All intentional ingredients are listed on the European's EINECS Inventory.

MEXICO

This product is considered to be corrosive according to Mexican Standard, Instruction No. 9, ANNEX 1.

STATE REGULATIONS

Not Available

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**REGULATIONS**

LOCAL REGULATIONS: Not Available

**16. OTHER INFORMATION**

REASON FOR ISSUE: New format with additional information.

APPROVED BY: William T. Stewart TITLE: Product Stewardship Manager

INFORMATION CONTACT: Product Stewardship Analyst

**REVISION SUMMARY**

This MSDS revision number was reset to #1 and replaces the April 08, 1997 issue.

**NFPA CODES**

FIRE: 1 HEALTH: 2 REACTIVITY: 1

**HMIS CODES**

FIRE: 1 HEALTH: 2 REACTIVITY: 1 PROTECTION: D

**MANUFACTURER SUPPLEMENTAL NOTES:**

**HAZARD WARNING!** This product belongs to a chemical family that HAS BEEN TESTED in combination with Trimethylolpropane, Trimethylolpropane derived products or their corresponding Trimethylolpropane homologs for toxicity of the thermal decomposition products in the absence of flame. Products in this chemical family PRODUCED NO SIGNIFICANT ADVERSE HEALTH EFFECTS in laboratory animals. However, there is a possibility that this thermal decomposition may produce bicyclic phosphates and/or phosphites in combination with certain other phosphorus compounds. Bicyclic phosphates and phosphites have acute neurotoxic properties and may cause convulsive seizures in laboratory test animals. Follow all precautionary measures outlined in this Material Safety Data Sheet and/or contact Albright & Wilson Americas.

**DATA SOURCES:**

Toxicological and ecological data based on Albright & Wilson UK Limited internal study reports.  
Product Health Hazard Review by Consultant Toxicologist, Dr. R. V. Blanke.

**MANUFACTURER DISCLAIMER:** Information given herein is offered in good faith as accurate, but without guarantee. Conditions of use and suitability of the product for particular uses are beyond our control; all risks of use of the product are therefore assumed by the user. Nothing is intended as a recommendation for uses which infringe valid patents or as extending license under valid patents. Appropriate warnings and safe handling procedures should be provided to handlers and users.

**RETURN TO MENU**

**Section H3: Environmental Fate Information**

(Note: Component Environmental Fate information is separated by colored paper)

**Hydrogen Peroxide**

**Acetic Acid**

**Peracetic Acid**

**Octanoic Acid**

**HEDP**

**000435**

**HYDROGEN PEROXIDE  
ENVIRONMENTAL FATE DATA**

ENVIRONMENTAL FATE DATA RETRIEVED FROM  
THE HAZARDOUS SUBSTANCES DATA BASE  
SYSTEM OF THE NATIONAL LIBRARY OF MEDICINE  
OR OTHER SPECIFIED SOURCES

HYDROGEN PEROXIDE

CAS RN: 7722-84-1

Natural Sources (HSDB) -

Gaseous hydrogen peroxide is recognized to be a key component and product of the earth's lower atmospheric photochemical reactions, both in a clean and polluted atmosphere. Atmospheric hydrogen peroxide is believed to be generated exclusively by gas-phase photochemical reactions. [IARC MONOGRAPHS 1972-PRESENT V36 p.291] \*\*PEER REVIEWED\*\*

Atmospheric Concentrations (HSDB) -

Measurements of hydrogen peroxide concentrations in the gas-phase and in cloud water were obtained in the vicinity of the USA Carolinas coast between late Jan and early Mar 1986. Gas phase concentrations, determined by a fluorometric method, were always less than 2.4 ppb and generally less than 1 ppb. Vertical profiles of hydrogen peroxide in the clear air around clouds and storm systems were highly variable. Concentrations of hydrogen peroxide in cloud water ranged from the detection limit of 0.3  $\mu\text{M}$  to 112  $\mu\text{M}$ , with higher values generally occurring in the vicinity of lightning activity. Hydrogen peroxide concentrations in cloud water were well below those calculated to be in Henry's law equilibrium with gas-phase concentrations of hydrogen peroxide in the cloudy air. [Barth MC et al; Tellus 41B (1): 61-9 (1989)] \*\*PEER REVIEWED\*\*

Routes of Exposure (HSDB) -

Inhalation of vapor or mist, ingestion, eye and skin contact. [SITTIG. HANDBOOK TOXIC HAZARD CHEM & CARCINOGEN 2 ED 1985, p. 510] \*\*PEER REVIEWED\*\*

Degradation (Laidler, K.J. Chemical Kinetics, 2nd. Ed., McGraw-Hill, 1965, pp 163-164 and 436)

Decomposition of hydrogen peroxide occurs slowly in the gas phase but is catalyzed efficiently by various metal ions in solution; some metals at levels as low as  $1 \times 10^{-8}$  Mole/L being effective in catalyzing the decomposition of hydrogen peroxide. Also, enzymatic degradation by the enzyme catalase (which occurs in animal and microfloral species) is very efficient with a turnover number of 5,000,000 molecules  $\text{H}_2\text{O}_2$ /minute per molecule of catalase. Thus, at a catalase level of 0.01 mMole/L (a common mid-range level for enzymatic species in organisms), approximately 5 mole/L-minute of hydrogen peroxide can be decomposed.

000436

**ACETIC ACID  
ENVIRONMENTAL FATE DATA**

ACETIC ACID  
CAS RN: 64-19-7

Environmental and Natural Sources (HSDB) -

Acetic acid occurs throughout nature as a normal metabolite of both plants and animals. Humans release acetic acid to the environment in a variety of waste effluents, in emissions from combustion processes, and in exhaust from gasoline and diesel engines. If released to the atmosphere, it is degraded in the vapor-phase by reaction with photochemically produced hydroxyl radicals (estimated typical half-life of 26.7 days). It occurs in atmospheric particulate matter in acetate form and physical removal from air can occur via wet and dry deposition. If released to water, acetic acid will biodegrade readily. If released to soil, it will also biodegrade readily. Evaporation from dry surfaces is likely to occur. Since acetic acid exists ubiquitously in the environment, the general population is continuously exposed to the compound. Primary routes of exposure to acetic acid are through oral consumption of foods and inhalation of air. Occupational exposure occurs through inhalation and dermal contact. (SRC)  
[CITATION ] \*\*PEER REVIEWED\*\*

It is found in unprocessed figs ... [FURIA. HDBK FOOD ADD 2ND ED 1972 , p. 226] \*\*PEER REVIEWED\*\*

Acetic acid ... is ... principal component of vinegars & pyroligneous acid. [FURIA. HDBK FOOD ADD 2ND ED 1972, p. 226]  
\*\*PEER REVIEWED\*\*

Occurs naturally in many fruit juices and in the stems and woody parts of plants [CONSIDINE, DM. CHEMICAL AND PROCESS TECHNOLOGY ENCYCLOPEDIA, (1974) p.21] \*\*PEER REVIEWED\*\*

... Occurs naturally in plant and animal tissues. ... Produced by fermentation of carbohydrates or by organic synthesis. ... /SRP: Ubiquitous in the environment/ [21 CFR 184.1005 (4/1/91)] \*\*PEER REVIEWED\*\*

Decomposition of solid biological wastes produces acetic acid which is readily metabolized by living organisms (1); acetic acid occurs as a normal metabolite in both plants and animals (1). It occurs naturally in various vegetation (2). [(1) Abrams E.F. et al; Identification of Organic Compounds in Effluents from Industrial Sources. USEPA-560/3-75-002 p. 3 (1975); (2) Graedel T.E. et al; Atmospheric Chemical Compounds. Sources, Occurrence and Bioassay. Orlando, FL: Academic Press p. 345 (1986)]  
\*\*PEER REVIEWED\*\*

Twenty-two acids in ground roast coffees and instant coffees were determined by GLC (gas liquid chromatography) of their silyl derivatives (after pre-separation by gel electrophoresis or isotachopheresis). The contribution to the total acidity (which was estimated by titration to pH 8 after cation exchange of the coffee solutions) was calculated for each individual acid. The acids contribute 67% (roast coffee) and 72% (instant coffee) to the total acidity. Citric acid (12.2% in roast coffee/10.7% in instant coffee), acetic acid (11.2%/3.3%) and the high MW acids (3%/9%) contribute to the total acidity. [Engelhardt U.F., Maier H.G.; Z Lebensmittel-Unters-Forsch 181 (1): 20-3 (1985)] \*\*PEER REVIEWED\*\*

000437

Manmade Sources (HSDB) -

Manufacturing source: beet sugar manufacturing; winery; vinegar manufacturing; textile mills; wood distillation plants. [VERSCHUEREN.HDBK ENVIRON DATA ORG CHEM 1983 , p. 143] \*\*PEER REVIEWED\*\*

Man made sources /of acetic acid have contributed/ 2.5 to 3.6 mg/l in domestic sewages. The average content of secondary sewage effluent is 0.130 mg/l. [VERSCHUEREN.HDBK ENVIRON DATA ORG CHEM 1983 , p. 144] \*\*PEER REVIEWED\*\*

Acetic acid ... /was/ present in 5 month-old compost of a town refuse. [DeVleeschauwer D, et al; BioCycle 22 (1): 44-6 (1981)] \*\*PEER REVIEWED\*\*

Acetic acid is released to the environment in waste emissions from the manufacture of various chemicals, explosives, lacquers, starch, sugars, wines and vinegar and from wood distillation plants and textile mills (1,2). Atmospheric emissions occur from combustion of biomass, plastics and refuse and in exhaust from gasoline and diesel engines (1,2,3). [(1) Abrams E.F. et al; Identification of Organic Compounds in Effluents from Industrial Sources. USEPA-560/3-75-002 p. 3 (1975); (2) Graedel T.E. et al; Atmospheric Chemical Compounds. Sources, Occurrence and Bioassay. Orlando, FL: Academic Press p. 345 (1986); (3) Kawamura K. et al; Environ Sci Technol 19: 1082-6 (1985)] \*\*PEER REVIEWED\*\*

Routes of Exposure (HSDB) -

Acetic acid can affect the body if it is inhaled or if it comes in contact with the eyes or skin. It can also affect the body if it is swallowed. [NIOSH OSHA. OCCUPAT HEALTH GUIDE CHEM HAZARDS. 1981 , p. 1] \*\*PEER REVIEWED\*\*

Acetic acid occurs ubiquitously and is a normal metabolite in animals; therefore, the general population is continually exposed to the compound. Primary routes of exposure to the general population are through consumption of foods and inhalation of air. Occupational exposure occurs through inhalation and dermal contact. (SRC) [CITATION] \*\*PEER REVIEWED\*\*

AIR INTAKE: Assume ambient atmospheric concns of 0.1-1.6 ug/cu m (1); 2-32 ug/day; WATER INTAKE: insufficient data; FOOD INTAKE: insufficient data(SRC). [(1) Kawamura K. et al; Environ Sci Technol 19: 1082-6 (1985)] \*\*PEER REVIEWED\*\*

NIOSH (NOHS Survey 1972-74) has statistically estimated that 1,400,824 workers are potentially exposed to acetic acid (1). NIOSH (preliminary NOES Survey 1981-1983) has statistically estimated that 340,218 workers are potentially exposed to acetic acid (2). [(1) NIOSH; National Occupational Hazard Survey (NOHS) (1974); (2) NIOSH; National Occupational Exposure Survey (NOES) (1983)] \*\*PEER REVIEWED\*\*

000438

Biodegradation (HSDB) -

Biological oxygen demand after 10 days at 20 deg C is: 82% biological oxidation in fresh water and 88% biological oxidation in sea water [VERSCHUEREN.HDBK ENVIRON DATA ORG CHEM 1983 , p. 144] \*\*PEER REVIEWED\*\*

Closed bottle test, 5-30 day 51-99% theoretical Biochemical Oxygen Demand BOD(1). Warburg respirometer, 30-day 60% theoretical BOD, acclimated sewage seed (2). Zahn-Wellens test, >90% degradation in 3 days using an activated sludge inocula (3). French Association for Standardization (AFNOR) T 90/103 test, 5-day 36% theoretical BOD, microbes from 3 polluted surface waters (4). Standard dilution BOD water, 5-day 57.7% theoretical BOD avg (5). Water-die away tests, 12.3%/hr in estuarine water, 1.0%/hr in Belgian coastal water, 0.06%/hr in open seawater (6). Standard dilution BOD water, 76-96% theoretical BOD in 5-20 days; Seawater dilution, 66-100% theoretical BOD in 5-20 days, sewage inocula (7). Batch aeration in sewage, 99.5% degradation in 24 hr (8). Warburg respirometer, 24-hr 40% theoretical BOD, activated sludge inocula (9). [(1) Fischer W.K. et al; Wasser-Und Abwasser-Forschung 7: 99-118 (1974); (2) Helfgott T.B. et al; An Index of Refractory Organics. USEPA-600/2-77-174 (1977); (3) Zahn R., Wellens H.; Z Wasser Abwasser Forsch 13: 1-7 (1980); (4) Dore M. et al; Trib Cebedeau 28: 3-11,(1975); (5) Heukelekian H., Rand M.C.; J Water Pollut Control Assoc 29: 1040-53 (1955); (6) Billen G. et al; Estuarine Coastal Marine Sci 11: 279-94 (1980); (7) Price KS et al; J Water Pollut Control Fed 46: 63-77 (1974); (8) Placak O.R., Ruchhoff C.C.; Sewage Works J 19: 423-40 (1947); (9) Malaney G.W., Gerhold R.M.; J Water Pollut Control Fed 41: R18-R33 (1963)] \*\*PEER REVIEWED\*\*

Warburg respirometer, 5-day 77% theoretical BOD, sewage inocula (1). Batch aeration, virtual loss of BOD in 6 hr, sealed domestic sewage inocula (2). Standard dilution BOD water, 5-day 81.3% theoretical BOD, 5-day 77.6% theoretical BOD (3). Standard dilution BOD water, 5-day 63.2% theoretical BOD, sewage inocula (4). Electrolytic respirometer test, 10-day 87% theoretical BOD (5). Laboratory-scale anaerobic digester, microbial decay coefficient of 0.283/day (6). Modified Organization of Economic Cooperation Development (OECD) protocol, 75% degradation in 14 days using garden soil as inocula, >90% degradation in 14 days using sediment from the Rhine River as inocula (7). Biofilm column study, 95% removal under aerobic conditions, 99% removal under methanogenic conditions (8). [(1) Dias F.F., Alexander M.; Appl Microbiol 22: 1114-8 (1971); (2) Hatfield R.; Ind Eng Chem 49: 192-6 (1957); (3) Takemoto S. et al; Suishitsu Odaku Kenkyu 4: 80-90 (1981); (4) Saito T. et al; Fresenius Z Anal Chem 319: 433-4 (1984); (5) Urano K., Kato Z.; J Hazardous Mater 13: 147-59 (1986); (6) Lin C. et al; Water Res 20: 385-94 (1986); (7) Kool HJ; Chemosphere 13: 751-61 (1984); (8) Bouwer E.J., McCarty P.L.; Ground Water 22: 433-40 (1984); (9) Strayer R.F., Tiedje J.M.; Appl Environ Microbiol 36: 330-40 (1978)] \*\*PEER REVIEWED\*\*

Abiotic Degradation (HSDB) -

The experimentally determined rate constant for the vapor-phase reaction of acetic acid with photochemically produced hydroxyl radicals has been reported to be  $0.6 \times 10^{-12}$  cu cm/molecule-sec at 25 deg C (1); the atmospheric half-life for this reaction can be estimated to be 26.7 days, assuming an average atmospheric hydroxyl radicals concn of  $5 \times 10^{-5}$  molecules/cu cm (1, SRC). The rate constant for the reaction of acetic acid with hydroxyl radicals in aqueous solution is approximately  $0.48-0.85 \times 10^{-8}$  L/mol-sec (2,3); if the hydroxyl radicals concn of sunlit natural water is assumed to be  $1 \times 10^{-17}$  moles/L (4), the half-life would be approximately 26-46 years (SRC). Carboxylic acids are generally resistant to aqueous environmental hydrolysis (5). [(1) Atkinson R.A.; Chem Rev 85: 60-201 (1985); (2) Anbar M., Neta P.; Int J Appl Radiation and Isotopes 18: 493-523 (1967); (3) Dorfman L.M., Adams G.E.; Reactivity of Hydroxyl Radical in Aqueous Solution, NSRD-NBS-46 Washington, DC: Natl Bureau of Standards (1973); (4) Mill T. et al; Science 207: 886-7 (1980); (5) Lyman W.J. et al; Handbook of Chemical Property Estimation Methods NY: McGraw-Hill p. 7-4 (1982)] \*\*PEER REVIEWED\*\*

000439

Other Biological / Environmental Data (HSDE) -

Acetic acid shows no potential for biological accumulation or food chain commination. [Environment Canada; Tech Info for Problem Spills: Acetic Acid (Draft) p.1 (1981)] \*\*PEER REVIEWED\*\*

Based on a log Kow of -0.17 (1), the ECF for acetic acid can be estimated to be <1 (2, SRC). This indicates that bioconcentration is not significant (SRC). [(1) Hansch C., Leo A.J.; Medchem Project Issue No. 26 Claremont CA: Pomona College (1985); (2) Lyman W.J. et al; Handbook of Chemical Property Estimation Methods NY: McGraw-Hill p. 5-4 (1982)] \*\*PEER REVIEWED\*\*

In 24 hr aqueous adsorption studies using montmorillonite and kaolinite clay adsorbents, 2.4-30.4% of added acetic acid was observed to be in the adsorbed phase (1). In adsorption studies using the adsorbent hydroxyapatite (a mineral which occurs in the environment as a result of the diagenesis of skeletal apatite), only 5% of added acetic acid (in aqueous solution) became adsorbed to the hydroxyapatite (2). Acetic acid has been noted to leach from biological disposal areas (3). [(1) Hemphill L., Swanson W.S.; Proc of the 18th Industrial Waste Conf, Eng Bull Purdue Univ, Lafayette IN 18: 204-17 (1964); (2) Gordon A.S., Millero F.J.; Microb Ecol 11: 289-98 (1985); (3) Abrams E.F. et al; Identification of Organic Compounds in Effluents from Industrial Sources. USEPA-560/3-75-002 p. 3 (1975)] \*\*PEER REVIEWED\*\*

Acetic acid has a pKa of 4.75 at 25 deg C (1); therefore, it will exist predominantly in the anionic form in the environment. The adsorption characteristics of an anionic species may be different from the neutral species, and cannot be predicted adequately without experimental data (SRC). [(1) Weast R.C.; CRC Handbook of Chemistry and Physics 66th ed, Boca Raton, FL: CR Press p. D-161 (1985)] \*\*PEER REVIEWED\*\*

The Henry's Law constant for acetic acid has been experimentally measured to range from  $1 \times 10^{-7}$  atm-cu m/mole at pH 4 to  $1 \times 10^{-9}$  atm-cu m/mole at pH 7 (1). These values of Henry's Law constant indicate that acetic acid will not volatilize significantly from water (2). [(1) Gaffney J.S. et al; Environ Sci Technol 21: 519-24 (1987) (2) Lyman W.J. et al; Handbook of Chemical Property Estimation Methods NY: McGraw-Hill p. 15-15 (1982)] \*\*PEER REVIEWED\*\*

The average content of secondary sewage effluent is 0.130 mg/l. [VERSCHUEREN.HDBK ENVIRON DATA ORG CHEM 1983 , p. 144] \*\*PEER REVIEWED\*\*

Acetic acid was qualitatively detected in wastewater effluents from publicly owned treatment works (POTW) in Decatur and Bensenville, IL (1). Acetic acid concns of 125 ppm were identified in wastewaters from a coal gasification facility in N Dakota (2). Wastewater from a shale oil process in Australia contained 140 ppm acetic acid (3). Acetic acid was detected in leachate from a sanitary landfill in Barcelona, Spain (4). Acetic acid has reportedly been detected in wastewater effluents from chemical, resin, and paper manufacturing plants, from various landfill leachates, and from sewage treatment facilities (5). [(1) Ellis D.D. et al; Arch Environ Contam Toxicol 11: 373-82 (1982); (2) Giabbai M.F. et al; Intern J Environ Anal Chem 20: 113-29 (1985); (3) Dobison K.R. et al; Water Res 19: 849-56 (1985); (4) Albaiges J. et al; Water Res 20: 1153-9 (1986); (5) Shackelford W.M., Keith L.M.; Frequency of Organic Compounds Identified in Water. USEPA-600/4-76-062 p. 47-8 (1976)] \*\*PEER REVIEWED\*\*

000440

**PERACETIC ACID  
ENVIRONMENTAL FACT DATA**

PERACETIC ACID  
CAS RN: 79-21-0

Environmental and Natural Sources (HSDB) -

Peracetic acid is formed naturally in the atmosphere through a series of photochemical reactions involving formaldehyde and photo-oxidant radicals. Due to its high water solubility, it can dissolve in clouds and rainwater. It has been identified as a constituent of acid rain. If released to the atmosphere or formed in the atmosphere, peracetic acid will most likely be removed physically by wet deposition processes. Degradation in the atmosphere is slow (estimated half-life for hydroxyl radical reaction is 445 days). If released to soil or water, peracetic acid is expected to react with organic materials, metal ions and complexes since it is chemically reactive. Occupational exposure to peracetic acid can occur through dermal contact and inhalation of vapor. (SRC) [CITATION] \*\*PEER REVIEWED\*\*

Peracetic acid can be formed naturally in the atmosphere through a series of photochemical reactions (1); for example, photo-oxidation of formaldehyde leads directly to the formation of hydroperoxyl radicals which react with peroxyacetyl radicals to form peracetic acid (1); the presence of anthropogenic nitric oxide decreases the formation rate of peracetic acid since it reacts preferentially with the species needed to form peracetic acid (1); therefore, atmospheric formation of peracetic acid will be greater at remote regions removed from sources of human pollution (1); the solubility of peracetic acid enables it to become a constituent of acid rain (1). [(1) Gaffney J.S. et al; Environ Sci Technol 21: 519-24 (1987)] \*\*PEER REVIEWED\*\*

Manmade Sources (HSDB) -

Peracetic acid's uses in textile and paper bleaching and in the production of epoxides and epoxy resins (1-2) could release the compound in production to the environment through wastewater effluents (SRC). [(1) Sheppard C.S., Mageli O.L.; Peroxides & Peroxy Compounds Organic In: Kirk-Othmer Encycl Chem Technol 3rd ed. NY: John Wiley & Sons 17: 60-2 (1982); (2) Hawley G.G.; The Condensed Chemical Dictionary 10th ed. NY: Van Nostrand Reinhold Co p. 786 (1981)] \*\*PEER REVIEWED\*\*

Environmental Fate (HSDB) -

TERRESTRIAL FATE: Peracetic acid is a chemically reactive compound (1) that can be expected to react with organic materials, metal ions and complexes that exist in the soil environment. Insufficient data are available to predict the relative importance of biodegradation in soil. An estimated Koc value of 7.5 suggests that non-ionized peracetic acid will leach readily in soil (2, SRC); however, concurrent reactivity with soil materials will probably negate the potential importance of leaching (SRC). [(1) Sheppard C.S., Mageli O.L.; Kirk-Othmer Encycl Chem Technol 3rd ed. NY: John Wiley & Sons 17: 60-1 (1982); (2) Lyman W.J. et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc p. 4-9 (1990)] \*\*PEER REVIEWED\*\*

AQUATIC FATE: Peracetic acid is a chemically reactive compound (1) that can be expected to react with organic materials, metal ions and complexes that exist in the aquatic environment. Insufficient data are available to predict the relative importance of biodegradation in water. Aquatic volatilization, adsorption to sediment, and bioconcentration are not expected to be important fate processes (SRC). [(1) Sheppard C.S., Mageli O.L.; Kirk-Othmer Encycl Chem Technol 3rd ed. NY: John Wiley & Sons 17: 60-1 (1982)] \*\*PEER REVIEWED\*\*

000441

ATMOSPHERIC FATE: Based upon a vapor pressure of 14.5 mm Hg at 25 deg C (1), peracetic acid is expected to exist almost entirely in the vapor-phase in the ambient atmosphere (2, SRC). It will degrade very slowly in an average ambient atmosphere by reaction with photochemically produced hydroxyl radicals (estimated half-life of 445 days) (3, SRC). Physical removal from air via wet deposition is likely to occur since peracetic acid is freely soluble in water (4, SRC); acidic precipitation can contain peracetic acid at nanomolar to low micromolar concentrations (5). [(1) Daubert T.E., Danner R.P.; Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation, NY: Hemisphere Pub Corp (1989); (2) Eisenreich S.J. et al; Environ Sci Technol 15: 30-8 (1981); (3) Atkinson R.; J Inter Chem Kinet 19: 799-828 (1987); (4) Merck; The Merck Index 10th ed. Rahway, NJ: Merck & Co p. 1028 (1983); (5) Gaffney J.S. et al; Environ Sci Technol 21: 519-24 (1987)] \*\*PEER REVIEWED\*\*

The rate constant for the vapor-phase reaction of peracetic acid with photochemically produced hydroxyl radicals has been estimated to be  $3.60 \times 10^{-14}$  cu cm/molecule-sec at 25 deg C which corresponds to an atmospheric half-life of about 445 days at an atmospheric concn of  $5 \times 10^{-5}$  hydroxyl radicals per cu cm (1, SRC). Organic peroxyacids are not noted for their stability (2); water-soluble peroxyacids (such as peracetic acid) hydrolyze slowly to the parent compound and hydrogen peroxide (2); peroxyacids are decomposed by a variety of metals, metal ions, and complexes (2); peracetic acid is a strong oxidizing agent (2). [(1) Atkinson R.; J Inter Chem Kinet 19: 799-828 (1987); (2) Sheppard C.S., Mageli O.L.; Kirk-Othmer Encycl Chem Technol 3rd ed. NY: John Wiley & Sons 17: 60-1 (1982)] \*\*PEER REVIEWED\*\*

#### Other Biological / Environmental Data (HSDB) -

Based upon an estimated Log Kow of -0.924(1), the BCF for peracetic acid can be estimated to be 0.12(SRC) from a recommended regression-derived equation (2). This indicates that bioconcentration in aquatic organisms is not important and in any case, peracetic acid would rapidly react with organic material (SRC). [(1) USEPA; Graphical Exposure Modeling System (GEMS). CLOGP (1987); (2) Lyman W.J. et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc p. 5-4 (1990)] \*\*PEER REVIEWED\*\*

Based upon a pKa of 8.20 at 25 deg C(1), peracetic acid can exist in both the ionized and non-ionized forms in environmental waters; the percentage of ionization depends upon pH with a 50% ionization occurring at pH 8.20; the sorption of ionized peracetic acid in soil cannot be predicted without experimental data (SRC). Based upon an estimated log Kow of -0.924 (2), the Koc for non-ionized peracetic acid can be estimated to be 7.5 (SRC) from a regression-derived equation (3); this estimated Koc suggests that peracetic acid is very highly mobile in soil(4); however, concurrent reactivity with soil materials will probably negate the potential importance of leaching (SRC). [(1) Dean J.A.; Lange's Handbook of Chemistry 13th ed. NY: McGraw-Hill Book Co p. 5-53 (1985); (2) USEPA; Graphical Exposure Modeling System (GEMS). CLOGP (1987); (3) Lyman W.J. et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc p. 4-9 (1990); (4) Swann R.L. et al; Res Rev 85: 23 (1983)] \*\*PEER REVIEWED\*\*

Peracetic acid has an experimentally measured Henry's Law constant of  $2.08 \times 10^{-6}$  atm cu m/mole at 25 deg C (1); a Henry's Law constant of this value indicates that volatilization from environmental waters is slow (2). Based on the Henry's Law constant, the volatilization half-life from a model river (1 m deep flowing 1 m/sec with a wind velocity of 3 m/sec) can be estimated to be about 15.5 days (2, SRC). Volatilization half-life from an model environmental pond (2 meters deep) can be estimated to be about 167 days (3, SRC). Peracetic acid has a relatively high vapor pressure of 14.5 mm Hg at 25 deg C (4) which suggests that some evaporation from dry surfaces can occur (SRC). [(1) Gaffney J.S. et al; Environ Sci Technol 21: 519-24 (1987); (2) Lyman W.J. et al; Handbook of Chemical Property Estimation Methods Washington, DC: Amer Chem Soc pp. 15-15 to 15-29 (1990); (3) USEPA; EXAMS II Computer Simulation (1987); (4) Daubert T.E., Danner R.P.; Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation, NY: Hemisphere Pub Corp (1989)] \*\*PEER REVIEWED\*\*

Routes of Exposure (HSDB) -

Occupational exposure to peracetic acid can occur through dermal contact and inhalation of vapor (1, SRC); personal protective equipment, including eye protection equipment, should be worn by persons handling the material (1). [(1) Parmeggiani L.; Encycl Occup Health & Safety 3rd ed Geneva, Switzerland: International Labour Office p. 44-5 (1983)] \*\*PEER REVIEWED\*\*

NIOSH (NOES Survey 1981- 1983) has statistically estimated that 1,729 workers are potentially exposed to peracetic acid in the USA (1). NIOSH (NOHS Survey 1972-1974) has statistically estimated that 1,683 workers are potentially exposed to peracetic acid in the USA (2). [(1) NIOSH: National Occupational Exposure Survey (NOES) (1983); (2) NIOSH: National Occupational Hazard Survey (NOHS) (1974)] \*\*PEER REVIEWED\*\*

000443

**OCTANOIC ACID  
ENVIRONMENTAL FATE DATA**

OCTANOIC ACID  
CAS RN: 124-07-2

Environmental and Natural Sources (HSDB) -

Reported as frequently occurring naturally in essential oils of: Cupressus torulosa, Cryptomer A Japonica, Andropogon  
iwarancusa, Cymbopogon javanensis, Camphor, Nutmeg, Lemon Grass, Lime, Tobacco (flowers), Artemissa herba-alba,  
Camomile, Hops...Apple aroma, Coconut oil...& wine... Lemon oil. [FENAROLI HDBK FLAVOR INGRED 2ND ED VOL2  
1975 , p. 442] \*\*PEER REVIEWED\*\*

Octanoic acid/ 8% in coconut oil [KIRK-OTHEMER ENCYC CHEM TECH 3RD ED 1978-PRESENT V21 p.164] \*\*QC  
REVIEWED\*\*

Synopsis -

Because it is a naturally occurring fatty acid octanoic acid will be readily utilized by animals, plants, and microbial organisms as a  
source of carbon and energy.

000444

SODIUM-1-OCTANE SULFONIC ACID: Carboxylic acid analog data provided

NONANOIC ACID [carboxylic acid analog of 1-octanesulfonic acid]  
CAS RN: 112-05-0

...AS AN ESTER IN OIL OF PELARGONIUM: REDTENBACHER, ANN 59: 41, 52, 54 (1846). [MERCK INDEX 9TH ED 1976, p. 916] \*\*PEER REVIEWED\*\*

...IN SEVERAL ESSENTIAL OILS, EITHER FREE OR ESTERIFIED: ROSE, GERANIUM, ORRIS, LITSEA CUBEBA, ARTEMISIA ARBORESCENS L, HOPS, CHAMAECYPARIS PISIFERA ENDL, EREMOCITRUS GLAUCA L, FRENCH LAVENDER, AND IN OAK MUSK. [FENAROLI HDBK FLAVOR INGRED 2ND ED VOL2 1975, p. 433] \*\*PEER REVIEWED\*\*

NO HAZARD IS LIKELY IN INDUSTRIAL USE. [ENCYC OCCUPAT HEALTH & SAFETY 1971, p. 29] \*\*PEER REVIEWED\*\*

CAPRIC ACID [1 carbon longer carboxylic acid analog of 1-octane sulfonic acid]  
CAS RN: 334-48-5

CAPRIC ACID, ISOLATED FROM AMERICAN ELM (ULMUS AMERICANA) SEEDS, WAS IDENTIFIED AS THE ANTIFUNGAL AGENT ACTIVE AGAINST THE DUTCH ELM DISEASE FUNGUS (CERATOCYSTIS ULMI) & SEVERAL OTHER FUNGI. [DOSKOTCH RW ET AL; PHYTOPATHOLOGY 65(5) 634-5 (1975)] \*\*PEER REVIEWED\*\*

OCTANOIC ACID, DECANOIC ACID, DODECANOIC ACID, TETRADECANOIC ACID, & HEXADECANOIC ACID (11.0-18.7% OF THE TOTAL ACIDS) WERE ISOLATED FROM THE NATURAL SEX PHEROMONES OF MALE MEDITERRANEAN FRUIT FLY (CERATITIS CAPITATA). [OHINATA K ET AL; J ENVIRON SCI HEALTH PART A A12(3) 67-78 (1977)] \*\*PEER REVIEWED\*\*

NATURAL FOOD OCCURANCES: ANISE, BUTTER ACIDS, OIL OF LIME, OIL OF LEMON. [CHEMICALS USED IN FOOD PROCESSING; NAS/NRC PUBL 1274 WASHINGTON DC (1965)] \*\*PEER REVIEWED\*\*

CAPRIC ACID (0.9%) WAS FOUND IN THE SEED OIL OF GARCINIA MANGOSTANA. [DAULATABAD CD, ANKALGI R.F.; J OIL TECHNOL ASSOC INDIA 10(2) 36-9 (1978)] \*\*PEER REVIEWED\*\*

Occurs as a glyceride in natural oils [HAWLEY. CONDENSED CHEM DICTNRY 10TH ED 1981 p.190] \*\*QC REVIEWED\*\*

Synopsis -

Since the fatty alkyl chain is oxidizable by living organisms it is expected that sodium 1-octane sulfonate will be used as an energy source as well as for its carbon and sulfur content by soil and water microflora.

000445

**HEDP  
ENVIRONMENTAL FATE DATA**

1-HYDROXY-1,1-DIPHOSPHONOETHANE  
CAS RN: 2809-21-4

Citations from the Chemical Abstracts Data Base -

- TI Properties of hydroxyethane diphosphonate affecting its environmental fate: degradability, sludge adsorption, mobility in soils, and bioconcentration
- AU Steber, J.; Wierich, P.  
CS Dep. Ecol., Henkel K.G.a.A., Duesseldorf, D-4000/1, Fed. Rep. Ger.  
SO Chemosphere (1986), 15(7), 929-45
- AB No indication of aerobic or anaerobic biodegradability of hydroxyethane diphosphonate (HEDP) [ \*\*\*2809-21-4\*\*\* ] was found. Nevertheless, the \*\*\*abiotic\*\*\* degradability of HEDP, particularly in natural waters under sunlight exposure, yielding acetate and inorg. phosphate excludes its environmental persistence. From adsorption and leaching studies a considerable HEDP elimination by sludge adsorption in sewage treatment plants and a characterization as moderately to little mobile in soils can be deduced. The results of a dynamic bioaccumulation test with fish show that HEDP has a very low bioconcn. potential.
- TI Distribution and elimination of HEDP in aquatic test systems  
AU Fischer, Klaus  
SO Water Res. (1993), 27(3), 485-93
- AB Basic reactions, including adsorption/desorption and photodegrdn., which influence the behavior and fate of chelating agents in sewage treatment processes and in aquatic ecosystems, were evaluated for HEDP. Freundlich consts. for the HEDP-sorption onto clay minerals, river sediments, and sewage sludges are mostly in the range between 500 and 3000. A remarkable desorption occurs only in strong acidic or higher concd. salt solns. Photodegrdn. is initiated in the presence of heavy metal ions and/or by maintaining acid pH conditions. The possibility of HEDP photodegrdn. in river water could be verified with a special equipment for the simulation of solar radiation. This investigation supports the assumption that discharged HEDP will be able to accumulate and persist in the aquatic \*\*\*environment\*\*\* if adsorption restricts the efficiency of the phosphonate photolysis.
- TI Distribution and photodegradation of chelating agents in \*\*\*environment\*\*\* -related test systems  
AU Fischer, Klaus  
SO GSF-Ber. (1992), 4/92, Ecol. Approaches Environ. Chem., 64-72
- AB The adsorption of HEDP and NTA on clay minerals, sediments, soils, and wastewater treatment sludges, desorption, and the effects of pH and Cu and Fe on the photodegrdn. of HEDP and NTA are described.

000446

TI Sorption of chelating agents (HEDP and NTA) onto mineral phases and sediments in aquatic model systems. Part I: sorption onto clay minerals

AU Fischer, Klaus

SO Chemosphere (1991), 22(1-2), 15-27

AB The fate of org. chelating agents in the aquatic \*\*\*environment\*\*\* may be detd. by reactions, which regulate the distribution of chems. between the solid and liq. phase. Esp. adsorption/desorption processes are important for the adjustment of the distribution equil. To assess the influence of such processes on the environmental fate of the phosphate substituting chelates 1-hydroxyethane-1,1-diphosphonic acid (HEDP) and nitrilotriacetic acid (NTA), adsorption studies were carried out in aquatic model systems, contg. different adsorbents like clay minerals, sediments and sewage sludges. -In the case of NTA, sorption strengths were kaolinite < engobe clay < bentonite.

ENVIRONMENTAL TOXICITY DATA RETRIEVED FROM  
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NAME - ACETIC ACID/RN - 64-19-7

ETXV - LC50 Fathead minnows > 315 mg/l/1 hr; 122 mg/l/24 hr; 92 mg/l/48 hr; 88 mg/l/72 hr; 88 mg/l/96 hr (static bioassay in reconstituted water at 18-22 deg C) [VERSCHUEREN.HDBK ENVIRON DATA ORG CHEM 1983 , p. 145] \*\*PEER REVIEWED\*\*

ETXV - LC50 Fathead minnows 175 mg/l/1 hr; 106 mg/l/24 hr; 106 mg/l/48 hr; 79 mg/l/72 hr; 79 mg/l/96 hr (static bioassay in reconstituted water at 18-22 deg C, pH < 5.9) [VERSCHUEREN.HDBK ENVIRON DATA ORG CHEM 1983 , p. 145] \*\*PEER REVIEWED\*\*

ETXV - TLm Culex (larvae) 1,500 mg/l/24-48 hr /Conditions of bioassay not specified/ [VERSCHUEREN.HDBK ENVIRON DATA ORG CHEM 1983 , p. 146] \*\*PEER REVIEWED\*\*

ETXV - LD0 Creek chub 100 mg/l/24 hr; Detroit river /Conditions of bioassay not specified/ [VERSCHUEREN.HDBK ENVIRON DATA ORG CHEM 1983 , p. 145] \*\*PEER REVIEWED\*\*

ETXV - LD100 Creek chub 200 mg/l/24 hr; Detroit river /Conditions of bioassay not specified/ [VERSCHUEREN.HDBK ENVIRON DATA ORG CHEM 1983 , p. 145] \*\*PEER REVIEWED\*\*

ETXV - TLm Daphnia magna (Arthropoda) 47 mg/l/24 hr /Conditions of bioassay not specified/ [VERSCHUEREN.HDBK ENVIRON DATA ORG CHEM 1983 , p. 145] \*\*PEER REVIEWED\*\*

ETXV - TLm Bluegill 75 mg/l/96 hr /Conditions of bioassay not specified/ [VERSCHUEREN.HDBK ENVIRON DATA ORG CHEM 1983 , p. 145] \*\*PEER REVIEWED\*\*

ETXV - TLm Lepomis macrochirus 100-1000 mg/l/24 hr /Conditions of bioassay not specified/ [VERSCHUEREN.HDBK ENVIRON DATA ORG CHEM 1983 , p. 145] \*\*PEER REVIEWED\*\*

ETXV - TLm Mosquito fish 251 mg/l/24-96 hr /Conditions of bioassay not specified/ [VERSCHUEREN.HDBK ENVIRON DATA ORG CHEM 1983 , p. 145] \*\*PEER REVIEWED\*\*

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- ETXV - Goldfish: lethal dose at 423 mg/l 20 hr, period of survival at pH 6.8 is 48 hr to 4 days at 100 ppm; period of survival at pH 7.3 is 4 days at 10 ppm [VERSCHUEREN.HDBK ENVIRON DATA ORG CHEM 1983 , p. 145] \*\*PEER REVIEWED\*\*
- ETXV - TLm Sunfish 75 mg/l/96 hr 18-20 deg C, soft water [Environment Canada; Tech Info for Problem Spills: Acetic Acid (Draft) p.76 (1981)] \*\*PEER REVIEWED\*\*
- ETXV - LC50 Shrimp 100-300 mg/l/48 hr aerated water [Environment Canada; Tech Info for Problem Spills: Acetic Acid (Draft)-p.76 (1981)] \*\*PEER REVIEWED\*\*
- ETXV - TLm Brine shrimp 22 mg/l/48 hr /Conditions of bioassay not specified/ [Environment Canada; Tech Info for Problem Spills: Acetic Acid (Draft) p.76 (1981)] \*\*PEER REVIEWED\*\*
- ETXV - Microcystis aeruginosa (algae) 90 mg/l toxic effect: cell multiplication inhibition [VERSCHUEREN.HDBK ENVIRON DATA ORG CHEM 1983 , p. 145] \*\*PEER REVIEWED\*\*
- ETXV - Scenedesmus quadricauda (green algae) 4000 mg/l toxic effect: cell multiplication inhibition [VERSCHUEREN.HDBK ENVIRON DATA ORG CHEM 1983 , p. 145] \*\*PEER REVIEWED\*\*
- ETXV - Entosiphon sulcatum (protozoa) 78 mg/l toxic effect: cell multiplication inhibition [VERSCHUEREN.HDBK ENVIRON DATA ORG CHEM 1983 , p. 145] \*\*PEER REVIEWED\*\*
- ETXV - Uronema parduczi Chatton-Lwoff (protozoa) 1350 mg/l toxic effect: cell multiplication inhibition [VERSCHUEREN.HDBK ENVIRON DATA ORG CHEM 1983 , p. 145] \*\*PEER REVIEWED\*\*
- ETXV - TLm Brine shrimp (Arthropoda) 42-32 mg/l/24-48 hr /Conditions of bioassay not specified/ [VERSCHUEREN.HDBK ENVIRON DATA ORG CHEM 1983 , p. 145] \*\*PEER REVIEWED\*\*

000449