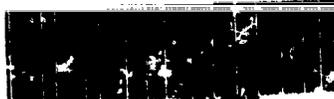


CODING FORMS FOR SRC INDEXING

Microfiche No.		OTS0001055	
New Doc ID	FYI-OTS-0794-1055	Old Doc ID	84950000004
Date Produced	02/13/89	Date Received	07/14/94
		TSCA Section	FYI
Submitting Organization		GREAT LAKES CHEM CORP	
Contractor			
Document Title		INITIAL SUBMISSION: LETTER FROM GREAT LAKES CHEM CORP TO CORP/USEPA SUBMITTING INFO RE HEXABROMOCYCLODODECANE AND BIS (TRIBROMOPHENOXY) ETHANE W/ATTCHMTS, DATED 2/13/89	
Chemical Category		HEXABROMOCYCLODODECANE; BIS (TRIBROMOPHENOXY)	



Great Lakes
Chemical Corporation



74I-0794-001055
INIT 07/14/94

200 4200 • HIGHWAY 13 N.W. • WEST LAFAYETTE, IN 47906 • PHONE: 317-467-6100 • FAX: 317-467-6204 • TELEX: 27-9428 • CABLE: GLAKCHEM LAFAYETTE

74I-0794-001055

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February 13, 1989



84958000004

Ms. Roberta Wedge
Dynamac
11140 Rockville Pyke
Rockville, MD 20852

Dear Ms. Wedge:

Copies of the following study reports which you requested are enclosed:

Hexabromocyclododecane (CD-75P)

Acute toxicity of HBCD to the bluegill sunfish.
HBCD - biodegradation study.
Partition coefficients of dicamba, endrin, VEL 3510 and several industrial chemicals and flame retardants.
Water solubility of several industrial chemicals, flame retardants and a herbicide VEL-3510.
Hydrolysis of Firemaster 100.

Bis(tribromophenoxy)ethane (FF-680)

Acute toxicity (TL50) study in the rainbow trout.
Fish bioaccumulation with 1,2-Bis(tribromophenoxy)ethane.
Biodegradability study with ¹⁴C-tagged MC-680 (November 1975).
Biodegradability study with ¹⁴C-tagged MC-680 (June 1976).
Partition coefficient of MC-680, chlorendic anhydride and chlorendic acid.
Water solubility of several flame retardants and industrial chemicals.
Solubility of MC-680 in various class solvents.
Photolysis of Firemaster 680.
Rate of hydrolysis studies.

From the nature of the studies requested, you are obviously evaluating the possible impact of environmental releases of these compounds. We are aware of only a very few reports in which these compounds have been identified in the environment. This is not surprising, considering the ways in which these chemicals are produced, distributed, and used.

Both of these chemicals are non-volatile substances which are manufactured in closed systems fully equipped with devices to control emissions. Wastes from the processes are either recycled or disposed of in approved hazardous waste landfills. Equipment now under construction and expected to start up in March of this year will eliminate the use of landfill disposal

Both CD-75 and FF-680 are used as flame retardant additives for plastics. Incorporation into the polymer matrix immobilizes these compounds and further diminishes the likelihood of environmental release.

I hope you find these reports useful. Please let me know if I can be of further assistance.

Sincerely,



Dennis L. McFadden
Product Safety
Coordinator

DLM:sb:78
Enclosures

CA-100-638

UCES Proj. No. 11506-03-77

THE ACUTE TOXICITY OF

HBCD
LOT #990-17

Hexabromocyclododecane
CAS# 3194-55-6

TO THE

BLUEGILL SUNFISH
Lepomis macrochirus Rafinesque

Prepared For

Velsicol Chemical Corporation
Chicago, Illinois

Prepared By

UNION CARBIDE ENVIRONMENTAL SERVICES
Union Carbide Corporation
Tarrytown, New York 10591

October 3, 1978

0005



UNION CARBIDE CORPORATION
ENVIRONMENTAL SERVICES

TARRYTOWN TECHNICAL CENTER
TARRYTOWN, NEW YORK 10591 • PHONE: (914) 345-3974

Client: Velsicol Chemical Corporation

Date: The test was conducted from September 7 through September 11, 1978.

Material: HBCD Lot #990-17

UCES Proj. No.: 11506-03-77

Summary: The 96 hour LC₅₀ for HBCD (Lot #990-17) to bluegill sunfish is greater than 100.0 mg/l. This value is based upon nominal concentrations of the chemical in soft reconstituted water.

Species: Bluegill sunfish

Length: 44 mm

Weight: 1.38 grams

Source: Nebraska

96 Hour LC₅₀: >100.0 mg/l

95% Conf. Limits: Not available

96 Hour Observed No Effect Level: 100.0 mg/l

Water Quality: Soft

Temperature: 20.3°C ± 0.7°C

pH: 7.50

Total Hardness as CaCO₃: 42 mg/l

96 Hr. LC₅₀ Ref. Toxicant p,p'-DDT: 4.03 (3.59 - 4.52) µg/l

Notebook Ref.: No. 4908, pages 59, 60

0006

INTRODUCTION

This study was conducted at the request of the Velsicol Chemical Corporation to determine the static acute toxicity of HBCD, Lot #990-17, to the bluegill sunfish. The test was performed at Union Carbide Environmental Services' (UCES) toxicity laboratory in Tarrytown, New York. HBCD is a white powder that is moderately soluble in acetone. HBCD formed a fine white precipitate in the stock solution which was suspended by agitation for dispensing into the test vessels. A white flocculate was formed on the surface of the water in all test concentrations upon addition of the stock.

The bluegill sunfish, Lepomis macrochirus Rafinesque, is a warm-water fish usually found in ponds, lakes and sluggish streams with bottoms of sand, gravel or mud. They feed on a variety of aquatic organisms including fish eggs, small fish, snails, insects and amphipods. Bluegills prefer temperatures above 20°C and can tolerate a wide pH range. Because of their wide geographic distribution, temperature requirements, and importance as a food web organism, the bluegill sunfish has been recommended by the Committee on Methods for Toxicity Tests with Aquatic Organisms (1975) as a bioassay organism.

METHODS

Dilution water used in all basic toxicity tests at the UCES laboratory is obtained from a well on the Tarrytown site, treated with a Continental Reverse Osmosis Water System (Model

3020) and deionized. After treatment, the water is reconstituted to the desired pH and hardness according to the procedures of Marking and Dawson (1973). For this test the soft reconstituted water was characterized as having a pH of 7.50, total hardness of 42 mg/l as CaCO₃, total alkalinity of 31 mg/l as CaCO₃, and a specific conductance of 160 µmhos/cm. Hardness and alkalinity were determined according to standard analytical procedures (American Public Health Association, 1976), pH with an ORION pH Meter, conductivity with a YSI Conductivity Bridge and dissolved oxygen with a YSI Oxygen Meter.

Five concentrations, a control and solvent control were used in determining the toxicity of HBCD, Lot #990-17, to bluegill sunfish. Test methodology followed recommended bioassay practices (U.S. Environmental Protection Agency, 1975) with the exception that replicate concentrations were not used. Fresh stock solution for the test was prepared by weight to a precision of 0.1 mg and diluted to volume in volumetric glassware with reagent grade acetone. The test was conducted in 19.6 liter, chemically clean glass jars containing 15 liters of water. The test was started by introducing the toxicant into test vessels containing dilution water, thoroughly mixing, and then introducing the fish. The amount of solvent in the solvent control equalled that amount used in the highest concentration.

Bluegill sunfish were obtained from a commercial hatchery in Nebraska and were maintained in the UCES laboratory at 22°C

According to the procedures of Brauhn, Schoettger and Mueller (1975). Mortalities in the stock culture over a one month period were less than two percent. Bluegill sunfish at the time of testing were approximately 4 months old and had a mean (10 organisms) length of 44 mm and a mean weight of 1.38 grams. Fish used in this test were randomly selected from the stock culture and acclimated to the test water for 24 hours prior to testing. Forty-eight hours before initiating the test the fish were taken off feed. Ten individuals were placed in each of the 19.6 liter test vessels. Biological loading was 0.92 g/l.

Dissolved oxygen and pH were determined initially and every 48 hours thereafter for the control, solvent control, high, medium and low toxicant concentrations. Water bath temperature was determined initially and at 48 hour intervals subsequent to the initiation of the test. In addition to obtaining the above chemical and physical parameters, abnormal behavioral responses of the test fish were noted and recorded at 24 hour intervals.

The concentration of toxicant lethal to 50% of the population (LC_{50}) and 95% confidence limits could not be determined due to the absence of mortalities. Test results were based upon nominal concentrations of the test material in soft reconstituted water. The no effect level was determined at the 96 hour exposure period. This value is based upon the absence of

abnormal behavior and may not necessarily be related to death.

RESULTS

The 96 hour LC_{50} for HBCD, Lot #990-17, to bluegill sunfish is >100.0 mg/l. Test results are presented in Table 1. The chemical and physical parameters monitored during the test are presented in Table 2. Behavioral observations made during the test indicated no observable abnormal behavior in any concentration throughout the test.

It should be noted that LC_{50} values may vary with different species, temperatures and water qualities.

Table 1 - Percent Mortalities and LC₅₀ Values

Client: Velsicol Chemical Corporation
 Test Material: HBCD, Lot #990-17
 Test Organism: Bluegill Sunfish

	Control	Solvent Control	Percent Mortality				
			Test Material, Nominal Conc. mg/l				
			10.0	18.0	32.0	56.0	100.0
24 hour	0	0	0	0	0	0	0
48 hour	0	0	0	0	0	0	0
96 hour	0	0	0	0	0	0	0

LC₅₀ Values

LC ₅₀ mg/l	24 Hour	48 Hour	96 Hour
95% Confidence Limits	>100.0	>100.0	>100.0
Low	N.A.	N.A.	N.A.
High	N.A.	N.A.	N.A.

N.A. = Not available due to absence of mortalities.
 The 96 hour observed no effect level is 100.0 mg/l.

Table 2 - Physical and Chemical Parameters

Client: Velsicol Chemical Corporation
 Test Material: HBCD, Lot #990-17
 Test Organism: Bluegill Sunfish

Dilution Water

pH	Specific Conductance µmhos/cm	Average Temperature °C	Total Hardness mg/l as CaCO ₃	Total Alkalinity mg/l as CaCO ₃
7.50	160	20.3 ± 0.7	42	31

Dissolved Oxygen, mg/l

	Control	Solvent Control	Test Material, Nominal Conc. mg/l	
			Test Material	Nominal Conc. mg/l
Initial	8.5	8.5	10.0	32.0
48 hour	7.3	7.2	8.6	8.5
96 hour	4.4	2.5	6.8	7.0
			2.2	1.9

pH

	Control	Solvent Control	Test Material, Nominal Conc. mg/l	
			Test Material	Nominal Conc. mg/l
Initial	7.50	7.49	10.0	32.0
48 hour	6.90	6.88	7.49	7.49
96 hour	7.07	6.90	6.87	6.85
			6.89	6.85

References

American Public Health Association. 1976. Standard Methods for the Examination of Water and Wastewater, 14th ed. New York. 1193 pp.

Brauhn, J. L., R. A. Schoettger and L. H. Mueller. 1975. Acquisition and Culture of Research Fish: Rainbow Trout, Fathead Minnows, Channel Catfish and Bluegills. EPA-660/3-75-001. 45 pp.

Committee on Methods for Toxicity Tests with Aquatic Organisms. 1975. Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. EPA-660/3-75-009. 61 pp.

Marking, L. L. and V. K. Dawson. 1973. Toxicity of Quinaldine Sulfate to Fish. Invest. Fish Control No. 48. U.S. Fish Wildl. Serv., Washington, D.C. 8 pp.

0013

Report Prepared By

Charles W. Calmbacher
Charles W. Calmbacher
Aquatic Toxicologist

Report Approved By

Algirdas G. Vilkas
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Aquatic Toxicology

Report Approved By

Curt Hutchinson
Curt Hutchinson
Manager
UNION CARBIDE CORPORATION
ENVIRONMENTAL SERVICES

October 3, 1978

MICHIGAN CHEMICAL CORPORATION

658

INTER-OFFICE MEMORANDUM

TO: L. H. Hahn

DATE: March 26, 1973

cc: A. F. Korst
R. C. Kamatz
C. File

*Hexabromocyclododecane
CAS# 3194-55-6*

VELSICOL CHEMICAL CORPORATION
BIOLOGICAL INDEXING SYSTEM

FROM: F. N. Trivedi

B. I. S. 18571
ORIGINAL COPY DO NOT REMOVE

SUBJECT: HBCD - Biodegradation Study

ORIGINAL RECORD
DO NOT REMOVE

PAGE.....OF.....PAGES

The biodegradability of hexabromocyclododecane (HBCD) was investigated at WARF Institute. They sent us benzene extracts of HBCD representing 0, 1, 5, and 7 days' exposure to bacterial medium. The 0 day samples were repeated (1) and 15 days' exposure samples were derived from this run. The following table indicates the total information derived from the study at WARF.

Analysis Date	Exposure	HBCD Content: In PPM	
		Blank	Sample
1/5/73	0 Day	None Detected	None Detected
	1 "	" "	0.2965
	5 "	" "	0.6690
	7 "	" "	0.4820
1/19/73	0 " (Repeat)	" "	1.1126
3/23/73	15 "	" "	0.5663

Attached to this memorandum is a graph representing the above figures. It appears from the data that HBCD is biodegrading to a certain extent.

(1) MCC, ICM, F. N. Trivedi to L. H. Hahn, January 23, 1973

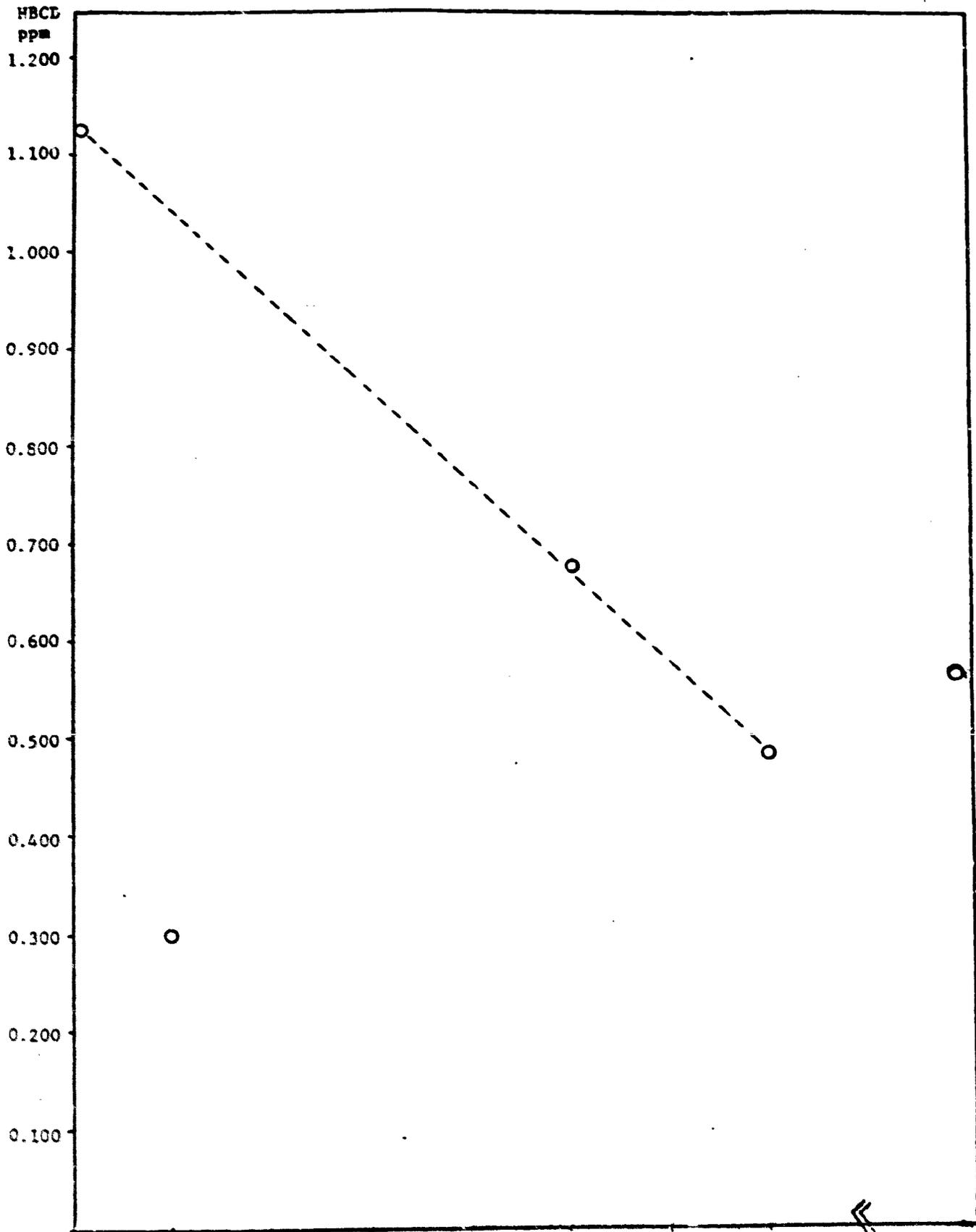
(Signature)

P. N. Trivedi

FNT:pr

Attachment

BIODEGRADATION OF HEXABROMOCYCLODODECANE



00-15

MICHIGAN CHEMICAL CORPORATION

INTER-OFFICE MEMORANDUM

MC-638

TO: L. R. Eaha

DATE: January 23, 1973

cc: A. F. Kerst
R. C. Nameta
C. File ✓

FROM: P. M. Trivedi

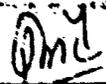
SUBJECT: HBCD - Biodegradation Study

The biodegradability of hexabromocyclododecane (HBCD) was investigated at WAMP Institute. They sent us benzene extracts of HBCD representing 0, 1, 5 and 7 days' of exposure to bacterial medium. We did not observe the presence of HBCD in the 0-day sample that should have the concentration of ~ 1.5 ppm HBCD. WAMP was contacted for this anomaly; and as a result, the 0-day experiment was repeated. The following table indicates the total information derived from the study at WAMP.

Analysis Date	Exposure	HBCD Content in ppm	
		Blank	Sample
1/5/73	0 Day	None Detected	None Detected
	1 "	" "	0.417 & 0.176
	5 Days	" "	0.653 & 0.675
	7 "	" "	0.497 & 0.467
1/19/73	0 Day (Repeat)	" "	1.1223 & 1.1029

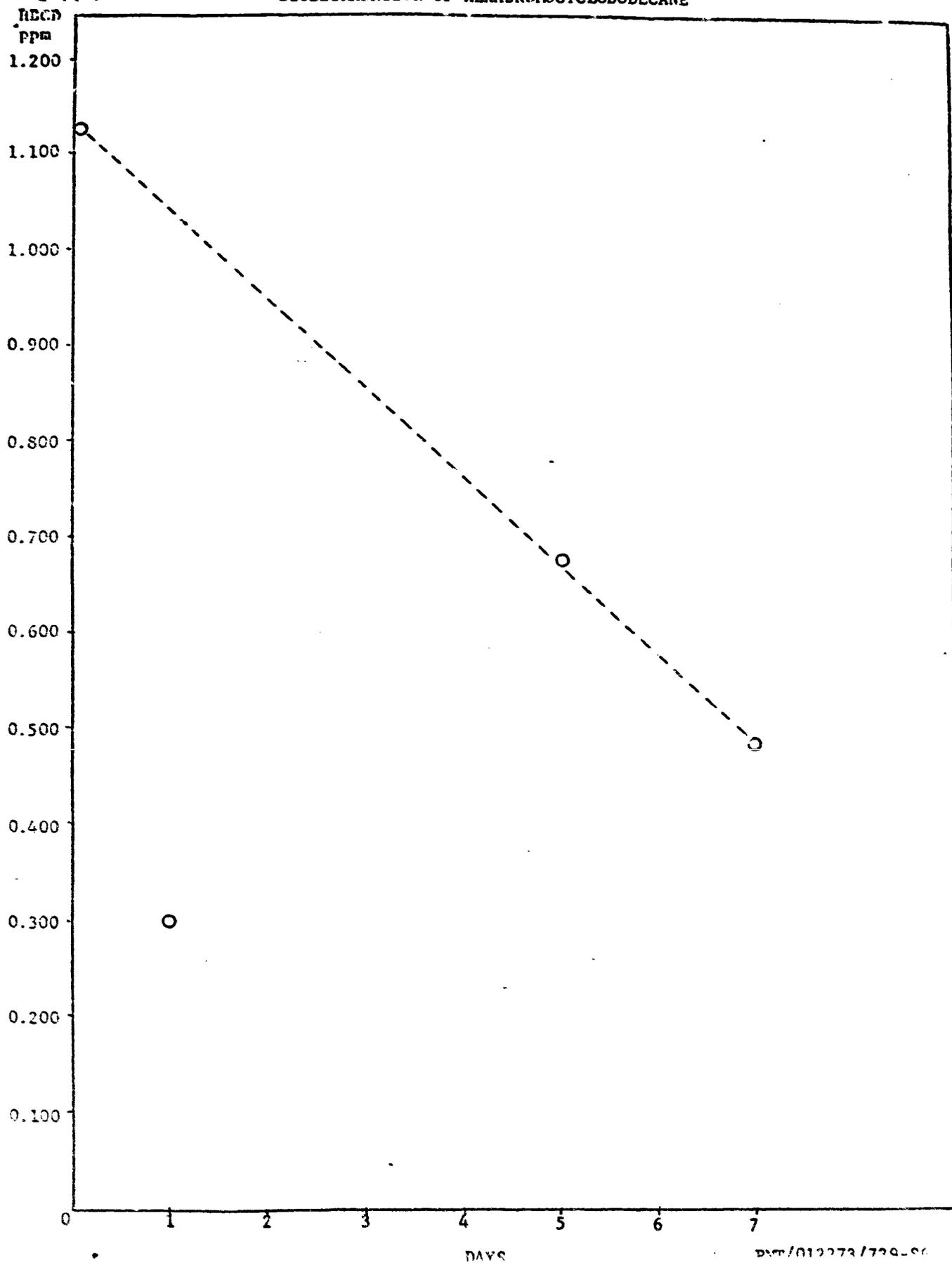
Attached to this memorandum is a graph representing the average of the above figures. The HBCD content at a lower concentration in 1-day sample in comparison to 5th & 7th day samples may be attributed to insufficient extraction and/or procedural error. It appears from the data that HBCD is biodegrading.

We are in the process of acquiring equipment to set up a biodegradation study unit. Microbial cultures have been gathered and are undergoing acclimation. The establishment of such an arrangement will let us have control over biodegradation studies and gain experience in testing these and other products.


P. M. Trivedi

PC:par

BIODEGRADATION OF HEXABROMOCYCLODODECANE



RETURN TO VAULT FILE

CN-10-0638

CONFIDENTIAL

VELSICOL CHEMICAL CORPORATION

LABORATORY REPORT

SUBJECT: Partition coefficient of dicamba, endrin
VEL 3510 and several industrial chemicals
and flame retardants

UNITERM NO: 5
480068/480048/414648/482308
PROJECT NO: 482108/484088/426918/482448

REPORT NO: 6/ 4/ 1/ 4/ 3/ 1/ 1/ 2

AUTHOR: C. C. Yu

SECTION: Environmental Sciences

DATE TYPED: September 7, 1979

COPIES TO:

PERIOD COVERED: July 1978 to August 1979

- L. G. Nickell
- D. M. Whitacre
- D. Y. Takade
- F. A. Daniher
- R. W. Atwell
- Y. H. Atallah
- C. C. Yu
- Vault (2)

WORK DONE BY: P. L. Thomas and C. C. Yu

SUPERVISOR: Y. H. Atallah

DEPARTMENT HEAD: D. Y. Takade

REFERENCES: Notebook no. 3680, pp 13-82

Notebook no. 3711, pp 30-60, 72-74

Notebook no. 4266 p 43

LOAN OUT

OBJECT: To determine the partition coefficient of several chemicals in n-octanol/water system.

SUMMARY: The partition coefficients in n-octanol/water system for several chemicals were determined. Each compound was measured in 2 concentrations using ¹⁴C-labeled materials. The averages of the partition coefficients for each compound are as follows: dicamba (0.1), endrin (2,704), Vel-3510 (64), benzyl alcohol (13), n-butyl benzoate (422), Benzoflex 245 (596), Benzoflex 988 (455), FM-100 (1,841), dicyclopentadiene (25), and benzo-trichloride (30).

Hexabromocyclododecane
CAS# 3194-55-6

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SIGNATURE *Ch. C. Yu*

INTRODUCTION

The partition coefficient of a given chemical in an organic/water system may serve as an indicator for the bioaccumulation potential of the chemical in aquatic environments (1). Therefore, the partition coefficients of dicamba, endrin, Vel 3510 and several industrial chemicals and flame retardants were determined to assist in the environmental evaluation of these chemicals.

MATERIALS AND METHODS

Chemicals:

¹⁴C dicamba was synthesized by New England Nuclear, Boston, Massachusetts.
¹⁴C endrin was obtained from California Bionuclear Corp., Sun Valley, California.
¹⁴C benzyl alcohol was synthesized by Pathfinder Laboratory, Inc., St. Louis, Missouri.
Other ¹⁴C chemicals were synthesized by Medwest Research Institute, Kansas City, Missouri.
Radiochemical purity of all ¹⁴C compounds was greater than 98% except benzotrichloride (96%). The major impurity was ¹⁴C benzoic acid (4%). The labeling position and specific activity of these ¹⁴C compounds were as follows:

Dicamba:	3,6-Dichloro- <i>o</i> -anisic acid-(phenyl-UL- ¹⁴ C), 6.49 mCi/mmole.
Endrin:	Hexachloroepoxyoctahydro-endo, endo-dimethanonaphthalene-(1,2,3,4,10- ¹⁴ C), 5.2 mCi/mmole.
Benzyl alcohol:	phenyl-UL- ¹⁴ C, 14.4 mCi/mmole.
n-Butyl benzoate:	phenyl-UL- ¹⁴ C, 10.2 mCi/mmole.
Benzoflex 245:	Diethyleneglycol dibenzoate-(phenyl-UL- ¹⁴ C), 4.2 mCi/mmole.
Benzoflex 988:	Dipropyleneglycol dibenzoate-(phenyl-UL- ¹⁴ C), 12.78 mCi/mmole.
FM-100 (HECD):	Hexabromocyclododecane-(UL- ¹⁴ C), 3.6 mCi/mmole.
Benzotrichloride:	phenyl-UL- ¹⁴ C, 10.2 mCi/mmole.
Dicyclopentadiene:	X- ¹⁴ C, 7.5 mCi/mmole.
Vel-3510:	1-β,β-dimethoxyethyl-1-methyl-3-(5-tert-butyl-1,3,4-thiadiazol-2- ¹⁴ C-2-yl) urea, 9.54 mCi/mmole.

Methods:

The methods described by Leo, Hansch and Elkins (1971) (Reference 2) were followed. Each chemical was studied at 2 concentrations. Each concentration was duplicated. A suitable amount of ¹⁴C chemical (between 0.15 and 0.7 μCi) was delivered to a 15 ml centrifuge tube. The solvent was evaporated completely under nitrogen, and then 2 ml of n-octanol (Mallinckrodt, Inc.) was added to dissolve the ¹⁴C material. Then 5-10 ml of distilled water was added to the tube and the tube was capped with a glass stopper. Each tube was inverted 200 x in about 5 min. and then was centrifuged at 3,000 rpm for 15 min. (International Equipment Co., Model CS). After centrifugation, duplicate 0.2 ml of the n-octanol phase were taken for radioassay. The remaining organic layer was completely removed using a Pasteur pipet. The duplicate 1 to 4 ml of the aqueous layer were taken for radioassay.

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Radioassay:

All samples were counted in Aquasol® scintillation solution (New England Nuclear) using Searle Mark III Liquid Scintillation System Model 6880 counter. An external standard pulse method was used to determine sample quenching. Counting efficiency, usually between 85-88%, was determined by an on-line computation program.

RESULTS

The concentrations of the chemicals in each phase were calculated (Table 1). The partition coefficients were also calculated from the ratio of the concentration in n-octanol and water (Table 1).

References Cited

1. Brock, N., D. R. Branson, and G. E. Blau. 1974. Partition Coefficient to Measure Bioconcentration Potential of Organic Chemicals in fish. Environ. Sci. and Tech., 8:1113.
2. Leo, A., C. Hansch, and D. Elkins. 1971. Partition Coefficients and their uses. Chem. Rev., 71: 537-538.

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Table 1. Partition coefficients of dicamba, endrin, endosulfan and several industrial chemicals and flame retardants.

Compound	Concentration (ppm) ^{1/}		Partition coefficient ^{2/}	Average Partition coefficient of I & II	
	in n-octanol	in water			
Dicamba	IA	0.0874	0.840	0.10	
	IB	0.0654	0.864		
	Average				0.09
	IIA	0.326	2.65		0.12
	IIB	0.178	2.62		0.07
	Average				0.10
Endrin	IA	16.95	0.007	2440	
	IB	18.67	0.007	2455	
	Average			2448	
	IIA	56.50	0.018	3016	
	IIB	56.61	0.019	2903	
	Average			2960	
Methyl alcohol	IA	0.45	0.034	13	
	IB	0.46	0.035	13	
	Average			13	
	IIA	1.58	0.12	13	
	IIB	1.28	0.096	13	
	Average			13	
Methyl benzoate	IA	0.94	0.0029	317	
	IB	0.98	0.0031	310	
	Average			314	
	IIA	5.56	0.010	548	
	IIB	5.46	0.010	511	
	Average			530	
Zoflex 245	IA	1.72	0.0034	505	
	IB	1.94	0.0036	527	
	Average			516	
	IIA	5.68	0.0082	688	
	IIB	5.82	0.0087	665	
	Average			677	
Zoflex 988	IA	2.37	0.0052	450	
	IB	2.23	0.0051	437	
	Average			444	
	IIA	7.31	0.015	473	
	IIB	7.32	0.016	457	
	Average			465	

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Hexabromocyclohexane
 CAS# 3194-55-6
 Table 1 (continued)

Compound	Concentration (ppm) ^{1/}		Partition coefficient ^{2/}	Average partition coefficient of I & II
	in n-octanol	in water		
t-100 (NBOD)	IA	9.40	0.0061	1528
	IB	9.60	0.0067	1436
	Average			1482
	IIA	28.30	0.026	1051
	IIB	27.80	0.0083	3348
	Average			2200
isotrchloride	IA	0.60	0.021	28
	IB	0.61	0.023	26
	Average			27
	IIA	2.43	0.060	40
	IIB	2.49	0.092	27
	Average			34
cyclopentadiene	IA	0.13	0.007	18
	IB	0.15	0.006	26
	Average			22
	IIA	0.43	0.016	27
	IIB	0.40	0.014	29
	Average			28
VEL-3510	IA	2.65	0.042	62
	IB	2.56	0.040	63
	Average			63
	IIA	8.10	0.124	65
	IIB	7.99	0.126	63
	Average			64

^{1/} Each value in the table represents an average of 2 assays.

^{2/} Partition coefficient = concentration in n-octanol phase / concentration in aqueous phase.

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RETURN TO VAULT FILE

CN-10-0638

CONFIDENTIAL

VELSICOL CHEMICAL CORPORATION

LABORATORY REPORT

SUBJECT: Water Solubility of Several Industrial
Chemicals, Flame Retardants and a
Herbicide VEL-3510.

UNITERM NO: _____
482148/482308/482108/484088
PROJECT NO: 482668/426918/416668

REPORT NO: 2574/2/5/2/2

AUTHOR: C. C. Yu

SECTION: Environmental Sciences

DATE TYPED: October 16, 1979

COPIES TO: L. G. Nickell
D. M. Whitacre
F. A. Daniher
R. W. Atwell
Y. H. Atallah
C. C. Yu
Vault (2)

PERIOD COVERED: July 1978 to August 1979

WORK DONE BY: P. L. Thomas and C. C. Yu

SUPERVISOR: Y. H. Atallah

LOAN OUT

DEPARTMENT HEAD: D. M. Whitacre

REFERENCES: Notebook no. 3542, pp. 96-98
Notebook no. 3680, pp. 17-29, 87-91
Notebook no. 3711, pp. 58-63, 75-80
Notebook no. 4266, pp. 45-47.

CONFIDENTIAL

This document contains confidential and proprietary information of Velsicol Chemical Corporation which information should not be disclosed to anyone not an employee of Velsicol Chemical Corporation, its parent or subsidiary companies.

OBJECT: To determine the water solubility of several industrial chemicals, flame retardants and a developmental herbicide (VEL-3510).

SUMMARY: Solubilities of several industrial chemicals, flame retardants and a developmental herbicide VEL-3510 were determined at 3 temperatures using ¹⁴C-labeled compounds. The results are as follows (in ppm at 15°, 25° and 35°C respectively): benzyl alcohol (47,040, 44,626, 48,917), n-butyl benzoate (138, 77, 55), benzoflex 245 (49, 51, 54), Benzoflex 988 (16, 15, 6), FM-100 (0.0087, 0.0086, 0.0078), benzotrifluoride (92, 165, 149), dicyclopentadiene (40, 33, 34), and Vel-3510 (4,307, 5,168, 5,554).

Hexabromocyclododecane
CAS# 3194-55-6

SIGNATURE: Ching Chieh Yu

10124

INTRODUCTION

Water solubility of a given chemical may be related to its adsorption and leachability in soil, bioaccumulation in aquatic organisms and mobility in the environment. Thus the water solubility of a compound is one of the principle factors which determine the fate of this compound in the environment. This study reports on the water solubility of several industrial chemicals, flame retardants and a developmental herbicide.

MATERIALS AND METHODS

Chemicals

¹⁴C benzyl alcohol and VEL-3510 were synthesized by Pathfinder Laboratories, Inc., St. Louis, Missouri. All other ¹⁴C chemicals were synthesized by Midwest Research Institute, Kansas City, Missouri. Radiochemical purity of all ¹⁴C compounds except benzotrachloride was greater than 98%. Benzotrachloride was 96% radiochemically pure (4% ¹⁴C benzoic acid as impurity). The labeling position and specific activity of these ¹⁴C compounds were as follows:

Benzyl alcohol:	phenyl-UL- ¹⁴ C, 14.4 mCi/mmole.
n-Butyl benzoate:	phenyl-UL- ¹⁴ C, 10.2 mCi/mmole.
Benzoflex 245:	Diethyleneglycol dibenzoate-(phenyl-UL- ¹⁴ C), 4.2 mCi/mmole.
Benzoflex 988:	Dipropyleneglycol dibenzoate-(phenyl-UL- ¹⁴ C), 12.78 mCi/mmole.
FM-100 (HBCD):	Hexabromocyclododecane-(UL- ¹⁴ C), 3.6 mCi/mmole.
Benzotrachloride:	phenyl-UL- ¹⁴ C, 10.2 mCi/mmole.
Dicyclopentadiene:	(X- ¹⁴ C), 7.5 mCi/mmole.
VEL-3510:	18, 8-dimethoxyethyl-1-methyl-3-(5- <u>tert</u> -butyl-1,3,4-thiadiazol-2- ¹⁴ C-2-yl) urea, 9.54 mCi/mmole.

Method

The ¹⁴C labeled materials were diluted with the respective analytical reference standards to achieve a suitable specific activity (Table 1). Appropriate amounts of the diluted ¹⁴C chemicals in solution were placed in polyallomer centrifuge tubes (Beckman Cat. no. 326814). A total of 6 tubes were prepared for each compound. A gentle stream of nitrogen was used to remove all the solvent from the tubes. Then twenty ml of distilled water was added to each tube, and caps (Beckman Cat. no. 338906) were placed over each tube and tightened. Tubes were then wrapped with aluminum foil. Two tubes were placed in a shaker water bath at 15°C, another two tubes at 25°C, and the remaining 2 tubes at 35°C. The tubes were shaken overnight and then centrifuged at 12,000 x G (Beckman Model LS-50 Preparative Ultracentrifuge, Rotor type 50.2 Ti fixed angle, operated at 11,500 rpm) at respective temperature (i.e. 15°C, 25°C or 35°C) for 1 hr. After centrifugation, duplicate 2 ml of the solution were taken for radioassay.

Radioassay

All liquid samples were counted in Aquasol® scintillation solution (New England Nuclear). A Mark III Liquid Scintillation System, Model 6880 (Searle Analytical, Inc.) was used for radiocarbon counting. Sample quenching was determined by an external standard pulse method. Counting efficiency, usually between 70-85%, was determined by an on-line computation program.

RESULTS AND DISCUSSION

The water solubility data is shown in Table 1. Benzyl alcohol is fairly soluble in water (about 46,000 ppm). VEL-3510 is about 1/10 as soluble as benzyl alcohol. FM-100 is least soluble in water (about 0.008 ppm). Water solubilities of the remaining 5 compounds are between 10-150 ppm.

The water solubility of VEL-3510 steadily increase when temperature increase from 15°C to 35°C, while the opposite is true for n-butyl benzoate and benzoflex 988. The solubility of the remaining compounds is not sensitive to water temperature change in the tested range.

Table 1 Water solubility of several industrial chemicals, flame retardants, and a herbicide VEL-3510¹.
CAS # 37953-59-1

	Compounds							
	Benzyl alcohol	n-butyl benzoate	Benzoflex 245	Benzoflex 988	FM-100 (HBCD)	Benzotrifluoride	Dicyclo-pentadiene	VEL-3510
specific activity (dpm/ μ g)	0.14	12.15	137	122	12,454	52.3	58	0.92
Amount (μ g/tube)	3.14×10^6	4×10^4	4×10^3	4×10^3	39.8	1×10^6	1×10^6	4×10^3
Water solubility (ppm) ²								
15°C	I 47,371	186	49	18	0.0091	92	41	4,280
	II 46,709	90	48	14	0.0083	93	38	4,334
	Average 47,040	138	49	16	0.0087	92	40	4,307
25°C	I 45,768	66	51	15	0.0082	181	33	5,221
	II 43,484	87	50	14	0.0089	149	33	5,114
	Average 44,626	77	51	15	0.0086	165	33	5,168
35°C	I 48,714	51	55	6	0.0084	138	32	5,753
	II 49,119	59	53	6	0.0071	160	35	5,354
	Average 48,917	55	54	6	0.0078	149	34	5,554

1/ After 1 hour of centrifugation at 12,000 x G.

2/ Each value in the table represents the average of duplicate analyses.

INTER-OFFICE CORRESPONDENCE

VELSICOL CHEMICAL CORPORATION

DATE	January 3, 1979	
TO	F. A. Danther	MAIL NO. 0714
FROM	P. M. Wiegand	MAIL NO. 0714
SUBJECT	HYDROLYSIS OF FIREMASTER [®] 100	

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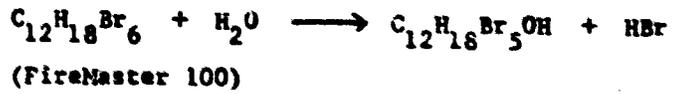
Hexabromocyclododecane PAGE..... OF..... PAGES
 CAS# 3194-55-6

An hydrolysis experiment on FireMaster 100 has been completed. The experiment was conducted as follows:

Nine samples of FireMaster 100, batch #180, were prepared for hydrolysis by placing approximately one gram of FireMaster 100 in each of nine bottles containing thirty mls of distilled water. The bottles were tightly capped and put on a shaker.

Samples were taken approximately twice weekly and the water tested for pH and bromide ion formation.

These two quantities were chosen as indicators of hydrolysis because the following hydrolysis reaction was considered most likely:



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After 900 hours (39 days) no bromide ion formation was detected in any of the samples. The detection limit of the method used was 200 ppm.

pH measurements did not show any significant trend when analyzed by linear regression analysis at the 95% confidence level.

One may conclude, therefore, that no significant hydrolysis occurs under the conditions of this experiment.

Hexabromocyclododecane
CAS# 3194-55-6

P. M. Wiegand
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PNW/plw

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