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Microfiche No.		OTS0001133	
New Doc ID	FYI-OTS-0794-1133	Old Doc ID	
Date Produced	10/10/88	Date Received	07/26/94
		TSCA Section	FYI
Submitting Organization		DOW CHEM CO	
Contractor			
Document Title		INITIAL SUBMISSION: LETTER FROM DOW CHEM CO TO USEPA REGARDING INFORMATION ON N,N-DIMETHYLDODECYLAMINE AND ETHANAMINE, N,N-DIETHYL WITH ATTACHMENTS, DATED 10/10/88	
Chemical Category		N,N-DIMETHYLDODECYLAMINE; ETHANAMINE, N,N-DIETHYL-	

FVI-0794-001133



THE DOW CHEMICAL COMPANY

MIDLAND, MICHIGAN 48674

October 10, 1988

Contains No CBI

Dr. Robert H. Brink, Executive Secretary
TSCA Interagency Testing Committee (TS792)
Environmental Protection Agency
401 M Street, S.W.
Washington, DC 20460

08 OCT 13 PM 1:38
OTS DOCUMENT CONTROL
OFFICE

Dear Dr. Brink:

Enclosed is information on N,N-Dimethyldodecylamine, CAS# 112-18-5, and Ethanamine, N,N-Diethyl-, CAS# 121-44-8. Both are listed in your February 24, 1988 Federal Register Notice (53 FR 5466) as candidates for review and possible recommendation for testing.

We hope that the information in this voluntary submission will be helpful to the Interagency Testing Committee.

Sincerely,

June W. Turley, Ph.D.
Research Associate
Regulatory Compliance
Health and Environmental Sciences
1803 Building



FVI-94-001133
INIT 07/26/94

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RHB

cbg

Enclosure



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1-DODECANAMINE, N,N-DIMETHYL-
CAS# 112-18-8

The chemical named above is neither a raw material in nor in the composition of any Dow product.

An acute mammalian toxicity study was done on this material in 1976 as part of an evaluation of its use in a Dow process. It was decided not to use it, and no additional work was done. A copy of the report of the study is enclosed.

J.W. Turley
10-3-88

9/29/76

**TOXICOLOGICAL PROPERTIES AND INDUSTRIAL HANDLING HAZARDS OF:
N,N-DIMETHYLDODECYLAMINE**

CAS No. 112-18-5

INFORMATIVE SUMMARY WITH CONCLUSIONS BASED ON THE SAMPLE RECEIVED. ADDITIONAL INFORMATION INCLUDING THE EFFECTS OF REPEATED EXPOSURE MAY BE REQUIRED AS SPECIFIC USES AND FORMULATIONS ARE DEVELOPED OR IF PROCESS CHANGES OCCUR.

A sample of N,N-dimethyldodecylamine bearing lot #21532-A, was submitted to the Toxicology Research Laboratory for toxicological evaluation and definition of industrial handling hazards. This clear colorless liquid will be used as a chemical reaction surfactant in a new process to produce a latex stabilizer.

Prolonged skin contact may result in moderate redness and swelling; repeated contact may also result in a moderate chemical burn. The material is not likely to be absorbed in acutely toxic amounts in a single contact, but may be absorbed in toxic amounts if skin contacts are repeated. Prolonged and repeated skin contact should be avoided. If skin contact occurs, wash contaminated skin with soap and water and clean contaminated clothes before re-use. Protective clothing, impervious to the material should be worn as required by circumstances.

Eye contact may result in moderate conjunctival irritation and slight corneal injury and iritis. These effects should heal in a week or so. If eye contact occurs, wash contaminated eyes with plenty of water for 15 minutes, then obtain medical attention. Chemical workers' goggles are recommended whenever eye contact is likely.

The single-dose oral LD50 in rats is between 1.25 & 2.5 g/kg which indicates a low acute oral toxicity. No problem is anticipated from ingestion incidental to industrial handling.

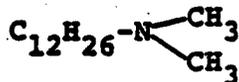
If this material is to be handled extensively, the effects of chronic exposure by skin absorption should be defined, and acute vapor inhalation studies should be conducted.

HEALTH & ENVIRONMENTAL RESEARCH
Industrial Hygiene & Toxicology Laboratories

THE DOW CHEMICAL COMPANY LIMITED

**DATA SHEET OF PROPERTIES, HEALTH HAZARDS, AND PRECAUTIONS
 FOR SAFE HANDLING OF MATERIALS**

MOLECULAR FORMULA $C_{14}H_{32}N$	NAME N,N-Dimethyldodecylamine
MOLECULAR WEIGHT 214.0	SYNONYMS Lauryldimethylamine;
STRUCTURAL FORMULA OR COMPOSITION	



PHYSICAL AND CHEMICAL PROPERTIES	BOILING POINT °C mmHg.	EXPLOSIVE LIMITS % VOL. IN AIR	FLASH POINT °C	IGNITION TEMP. °C	MELTING POINT °C	VAPOR PRESS. mmHg. 25°C.
	CORROSIVENESS (To Common Metals)			PHYSICAL STATE Liquid	COLOR Clear, colorless	
	CHEMICAL REACTIVITY				ODOR (Include Concentration in Air)	
	STABILITY (To pH Change, Heat, Light)					

TYPE OF CONTACT		CLASSIFICATION OF TOXIC PROPERTIES	
TOXIC PROPERTIES	EYE	<input type="checkbox"/> MAY CAUSE NO RESPONSE OR NO MORE THAN VERY SLIGHT TO SLIGHT TRANSITORY PAIN AND/OR SLIGHT TRANSIENT CORNEAL INJURY AND/OR IRRITATION OF THE EYELIDS.	<input type="checkbox"/> MAY CAUSE SOME PERMANENT LOSS OF VISION (THIS INCLUDES DAMAGE TO CORNEA OR INTERNAL INJURY WHICH IS INCOMPLETELY HEALED IN ONE WEEK.)
		<input checked="" type="checkbox"/> MAY CAUSE SUFFICIENT INJURY TO THE EYE TO RESULT IN LOSS OF TIME FROM WORK. (THIS INCLUDES DAMAGE TO THE CORNEA WHICH HEALS OR NEARLY HEALS IN A WEEK AND/OR CONSIDERABLE CONJUNCTIVAL IRRITATION WITH EDEMA.)	<input type="checkbox"/> VAPOR EXPOSURE MAY CAUSE SEVERE PAIN, LACRYMATION OR SERIOUS INJURY TO THE EYES.
	SKIN	<input type="checkbox"/> SINGLE PROLONGED EXPOSURE (HOURS) CAUSES NO EFFECT SEVERAL REPEATED PROLONGED EXPOSURES MAY OR MAY NOT CAUSE THE DEVELOPMENT OF SOME SLIGHT IRRITATION.	<input type="checkbox"/> SINGLE SHORT EXPOSURE (MINUTES) MAY CAUSE CONSIDERABLE IRRITATION AND/OR SINGLE PROLONGED OR FREQUENTLY REPEATED SHORT EXPOSURES CAUSE A BURN AND/OR MAY CAUSE SYSTEMIC INJURY, EVEN DEATH.
		<input checked="" type="checkbox"/> SINGLE PROLONGED EXPOSURE MAY CAUSE SOME REDDENING OF THE SKIN. REPEATED PROLONGED CONTACTS MAY CAUSE APPRECIABLE IRRITATION, POSSIBLY A MILD BURN AND/OR MAY CAUSE APPRECIABLE SYSTEMIC INJURY DUE TO ABSORPTION.	<input type="checkbox"/> AN EXPOSURE RAPIDLY CAUSES SEVERE BURNS AND/OR SERIOUS SYSTEMIC INJURY, EVEN DEATH.
DUST OR MIST	<input type="checkbox"/> NO SYSTEMIC INJURY EXPECTED. NO IRRITATION TO NOSE AND THROAT IN DUSTY OR MISTY ATMOSPHERES.	<input type="checkbox"/> DUSTY OR MISTY ATMOSPHERE PAINFUL TO NOSE AND THROAT (INTOLERABLE TO MOST PEOPLE) AND/OR EXPOSURE MAY CAUSE SERIOUS SYSTEMIC INJURY, EVEN DEATH.	
	<input type="checkbox"/> THROAT AND NOSE IRRITATION IN A DUSTY OR MISTY ATMOSPHERE IS PAINFUL BUT NOT INTOLERABLE AND/OR PROLONGED OR REPEATED EXPOSURES MAY CAUSE SYSTEMIC INJURY.	<input type="checkbox"/> SHORT EXPOSURE (MINUTES) MAY CAUSE DEATH OR SERIOUS SYSTEMIC INJURY.	
VAPOR <small>Tested at room temperature unless otherwise indicated.</small>	<input type="checkbox"/> EXPOSURES DO NOT CAUSE ANY EFFECTS OTHER THAN SOME VERY SLIGHT IRRITATION OR PAIN TO THE EYES OR RESPIRATORY PASSAGES AT THE MOST.	<input type="checkbox"/> EXPOSURES MAY CAUSE EXTREME DROWSINESS, AND/OR SERIOUS SYSTEMIC INJURY, AND/OR MAY CAUSE INTOLERABLE IRRITATION TO THE RESPIRATORY PASSAGES.	
	<input type="checkbox"/> SINGLE EXPOSURES EXCEEDING 1/2 HOUR, OR FREQUENTLY REPEATED EXPOSURES OF SHORTER DURATION, MAY CAUSE SLIGHT ANESTHESIA AND/OR SLIGHT SYSTEMIC INJURY, AND/OR CAUSE APPRECIABLE, BUT NOT INTOLERABLE, IRRITATION OF RESPIRATORY PASSAGES.	<input type="checkbox"/> SHORT EXPOSURES MAY CAUSE UNCONCIOUSNESS, AND/OR SERIOUS SYSTEMIC INJURY, INCLUDING DEATH.	
INGESTION	<input checked="" type="checkbox"/> AMOUNTS WHICH MAY BE SWALLOWED INCIDENTAL TO INDUSTRIAL HANDLING WILL NOT CAUSE INJURY, HOWEVER, IF SUBSTANTIAL QUANTITIES SHOULD BE SWALLOWED, MORE OR LESS SERIOUS EFFECTS MAY OCCUR.	<input type="checkbox"/> AMOUNTS WHICH MAY BE SWALLOWED INCIDENTAL TO INDUSTRIAL HANDLING AND USE MAY CAUSE SERIOUS INJURY.	

COMMENTS

N,N-Dimethyldodecylamine

DEGREES OF EXPOSURE RELATED TO TYPES OF OPERATION		PRECAUTIONS (SEE CODE BELOW)				
		EYES	SKIN	INHALATION*		INGESTION
				DUST OR MIST	VAPOR	
I NO CONTACT	CHARACTERIZED BY REMOTE OPERATION WITH EQUIPMENT ISOLATED FROM THE WORK AREA. THE PERSONS ENTERING ISOLATED AREAS WILL REQUIRE THE PERSONAL PROTECTION OUTLINED FOR IV BELOW.	A	A			A
II MINOR CONTACT	CHARACTERIZED BY CLOSED SYSTEMS WITH EQUIPMENT VENTED OUTSIDE THE WORK AREA. INSTRUMENT CONTROL, MECHANICAL HANDLING OF MATERIALS IN BULK. EXAMPLES ARE: CONTINUOUS REACTORS, STILLS AND FILTERS, ENCLOSED CONVEYORS, VENTILATED PACKAGING.	B	A			A
III OCCASIONAL DAILY CONTACT	CHARACTERIZED BY MANUAL HANDLING OF MATERIALS IN PACKAGES SUCH AS BAGS, DRUMS AND FIBERPAKS. VENTILATION MAY BE PROVIDED FOR SPECIFIC JOBS. MANY BATCH OPERATIONS FALL INTO THIS CATEGORY.	B	B			A
IV GROSS CONTACT LIKELY	CHARACTERIZED BY HAND OPERATION. EXAMPLES ARE: EMERGENCY REPAIRS, CLEANING EQUIPMENT, CLEANING FILTERS, TAKING CARE OF SPILLS, PACKAGING VOLATILE OR DUSTY MATERIALS WITHOUT VENTILATION, WHEELING AND TRAY DRYING.	D	D			A
EYE CONTACT		A NO EYE PROTECTION NEEDED. B USE SAFETY GLASSES WITHOUT SIDE SHIELDS. C USE SAFETY GLASSES WITH SIDE SHIELDS.		D USE CHEMICAL WORKERS GOGGLES. E USE GAS TIGHT GOGGLES OR A FULL FACE GAS MASK.		
SKIN** CONTACT		A A BATH AND CLEAN CLOTHES ONCE PER WEEK ALONG WITH THE USUAL WASHING AT MEALTIMES SHOULD BE ADEQUATE PRECAUTIONS. B GROSSLY CONTAMINATED CLOTHING AND SHOES MUST BE REMOVED NOT LATER THAN THE END OF THE WORK PERIOD AND MUST BE THOROUGHLY CLEANED BEFORE RE-USE. C REQUIRE SHOWER AT THE END OF THE WORK PERIOD AND CLEAN CLOTHING FROM THE SKIN OUT AT THE START OF EACH WORK DAY.		D CLOTHING SHOULD BE CHANGED AND SKIN WASHED PROMPTLY UPON ANY DETECTABLE CONTACT. EACH USE WILL REQUIRE SPECIAL CONSIDERATION TO DETERMINE SUITABLE PROTECTIVE DEVICES AND STANDARDS OF PERSONAL CLEANLINESS. E IMPERVIOUS CLOTHING SUCH AS RUBBER BOOTS, RUBBER APRONS, AND RUBBER GLOVES WILL BE REQUIRED. SPECIFIC ITEMS WILL BE DICTATED AS REQUIRED BY CIRCUMSTANCE.		
INHALATION	DUST OR MIST	A NO RESPIRATORY PROTECTION. B NO PROTECTION REQUIRED FOR EXPOSURE OF THIRTY MIN. DURATION OR LESS TO OBVIOUSLY DUSTY ATMOSPHERES. EXPOSURES OF LONGER DURATION WILL REQUIRE THE USE OF A DUST RESPIRATOR BEARING THE APPROVAL OF THE U.S. BUREAU OF MINES FOR THE USE WITH TOXIC DUSTS.		D ANY EXPOSURE TO OBVIOUSLY DUSTY ATMOSPHERES WILL REQUIRE A DUST RESPIRATOR BEARING THE APPROVAL OF THE U.S. BUREAU OF MINES FOR USE WITH TOXIC DUSTS. E ANY EXPOSURE TO DUSTY ATMOSPHERES WILL REQUIRE THE USE OF AN AIRLINE RESPIRATOR, BLOWER MASK, OR CHEMOX MASK.		
	VAPOR	A NO PRECAUTIONS NECESSARY. B NO PRECAUTIONS NECESSARY FOR SINGLE EXPOSURES OF LESS THAN 1/2 HOUR. LONGER SINGLE EXPOSURES, OR FREQUENTLY REPEATED EXPOSURES WILL REQUIRE A GAS MASK OR RESPIRATOR EQUIPPED WITH APPROPRIATE CANISTER.		C NO PRECAUTIONS NECESSARY FOR SINGLE EXPOSURES OF NO MORE THAN TEN MINUTES. LONGER EXPOSURES EITHER SINGLE OR REPEATED, WILL REQUIRE GAS MASK OR RESPIRATOR EQUIPPED WITH APPROPRIATE CANISTER. D C MASK WITH APPROPRIATE CANISTER REQUIRED AT ALL TIMES. E EVACUATE AREA AT ONCE AND ENTER ONLY WITH AIRLINE RESPIRATOR, BLOWER MASK OR CHEMOX MASK.		
INGESTION		A NO UNUSUAL PROCEDURES REQUIRED.		E FOOD AND TOBACCO SHOULD NOT BE PRESENT IN THE WORK AREA. HANDS AND FACE SHOULD BE WASHED BEFORE SMOKING AND EATING.		

COMMENTS **GOOD PRACTICE REQUIRES THAT GROSS AMOUNTS OF ANY CHEMICAL BE REMOVED FROM THE SKIN AS SOON AS IS PRACTICAL

*SUITABLE GAS MASK CANISTER
(See SLP Tok Bulletin #3)

Organic Vapor

SIGNED _____ CHECKED _____
 DATE 9/23/76 DATE 10/5/76



DOW CHEMICAL U.S.A.

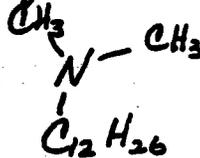
ENVIRONMENTAL HEALTH SERVICES

MIHLAND, MICHIGAN

REQUEST FOR PRELIMINARY TOXICOLOGICAL STUDIES

FILE

MOLECULAR FORMULA C₁₄H₂₇N	NAME N, N-Dimethyldodecylamine
MOLECULAR WEIGHT 214.0	SYNONYMS Lauryldimethylamine
STRUCTURAL FORMULA - OR COMPOSITION	



PHYSICAL AND CHEMICAL PROPERTIES	BOILING POINT	EXPLOSIVE LIMIT (% BY VOL. IN AIR)	FLASH POINT	IGNITION TEMP. °C	MELTING POINT °C	VAPOR PRESSURE mmHg, 50°C
	CORROSIVENESS (To Common Metals)	PHYSICAL STATE		COLOR		
	CHEMICAL REACTIVITY	STABILITY (To pH Change, Heat, Light)		ODOR (Include Concentration in air)		
	SOLUBILITY					

SAMPLE REFERENCE AND SOURCE

lot # 21532-A

REPORT TO ADDRESS

SUPERVISOR (Signature)	DATE	BLOG.
PRODUCT SAFETY COORDINATOR (Signature)	DATE	SU

DO NOT WRITE BELOW THIS LINE - COMPLETE INFORMATION ON REVERSE SIDE *copy to F*

SAMPLE RECEIVED BY TOXICOLOGY AND PROTOCOLS COMPLETED:

ESTIMATED COMPLETION DATE:

TEST	ANIMAL	SEX	SOLVENT	DOSE (g/kg)	ANIMALS ON TEST	TESTS DONE	ADDITIONAL WORK	DONE	TOX. RESULTS	PHONED TO DATE
ACUTE ORAL	RAT		CORN OIL	.063						
	GUINEA PIG		WATER	.126						
	RABBIT		UNDILUTED	.252						
	CHICK			.50						
				1.0						
				2.0						
				3.98						
EYE CONTACT	RABBIT		WATER	100%						
			PROPYLENE GLYCOL	10%						
				1%						
SKIN CONTACT REPEATED	RABBIT			100%						
			WATER	10%						
				1%						
SKIN CONTACT SINGLE EXPOSURE										
SENSITIZATION	GUINEA PIG									
SKIN ABSORPTION SINGLE EXPOSURE	RABBIT			.126						
				.252						
				.50						
				1.0						
				2.0						
				3.98						
ACUTE INHALATION RAT			SAT. VAPOR	<input type="checkbox"/>						
			PPM							
			PRESSURIZED CAN							
			AEROSOL							

return sample
MS A7
called Bob
9/27

REPORT DRAFTED _____

REPORT ISSUED _____

SAMPLE RETURNED _____

SAMPLE TO K STORAGE _____

SAMPLE DESTROYED _____

REASON OR NEED FOR TOXICOLOGICAL TESTS:

data hand. sheet

STAGE OF DEVELOPMENT:

RESEARCH BENCH PILOT PLANT SEMI PLANT PLANT REGISTRATION

PROPOSED AND POTENTIAL USE:

*to be used in
surfactant reactions*
*To be used as chemical reaction surfactant in a proposed
new process to produce a latex stabilizer*

METHOD OF HANDLING:

AMOUNTS TO BE HANDLED:

HUMAN EXPERIENCE IN HANDLING:

NOTES:

CHARGE NO. _____

MATERIAL

N,N-Dimethyldodecylamine

% SOLUTION IN:

UNDILUTED WATER CORN OIL

SPECIES

RAT GAVY RABBIT MOUSE MALE FEMALE

WEIGH OUT (OTHER)

CASE	DATE FED	ANIMAL MARKING	WEIGHT GM.	DOSE GM./KG.	DOSE CC.	ANIMAL WEIGHT (GM.)		DATE	
						9-3-76	9/15		
52-7	11:00 9/2/76	0	232	.316	0.004	244	292	336	} <i>Sal</i>
		01	208		0.085	218	259	304	
		10	211		0.086	237	<i>path</i>		
-8		11	200	.63	0.163	190	227	289	
		02	201		0.164	220	245	290	
		00	220		0.179	213	<i>path</i>		
-9		01	229	1.26	0.373	226	252	319	
		10	205		0.334	206	211	286	
		11	203		0.330	192	<i>path</i>		
-10		02	204	2.52	0.665	202	<i>Dead</i>		
		00	219		0.713	222	<i>9-5-76</i>		
		01	223		0.726	227	<i>path</i>		
-11		10	207	5.0	1.338	<i>7</i>	<i>D.O</i>		
		11	199		1.287	<i>5</i>	<i>9/3/76</i>		
		02	185		1.196	<i>dead</i>	<i>5 hrs</i>		

O.B. (u) (u) 484 O.B. O.B.

OBSERVATION BY

COMMENTS ON BACK OF THIS PAGE

SIGNED

DATE

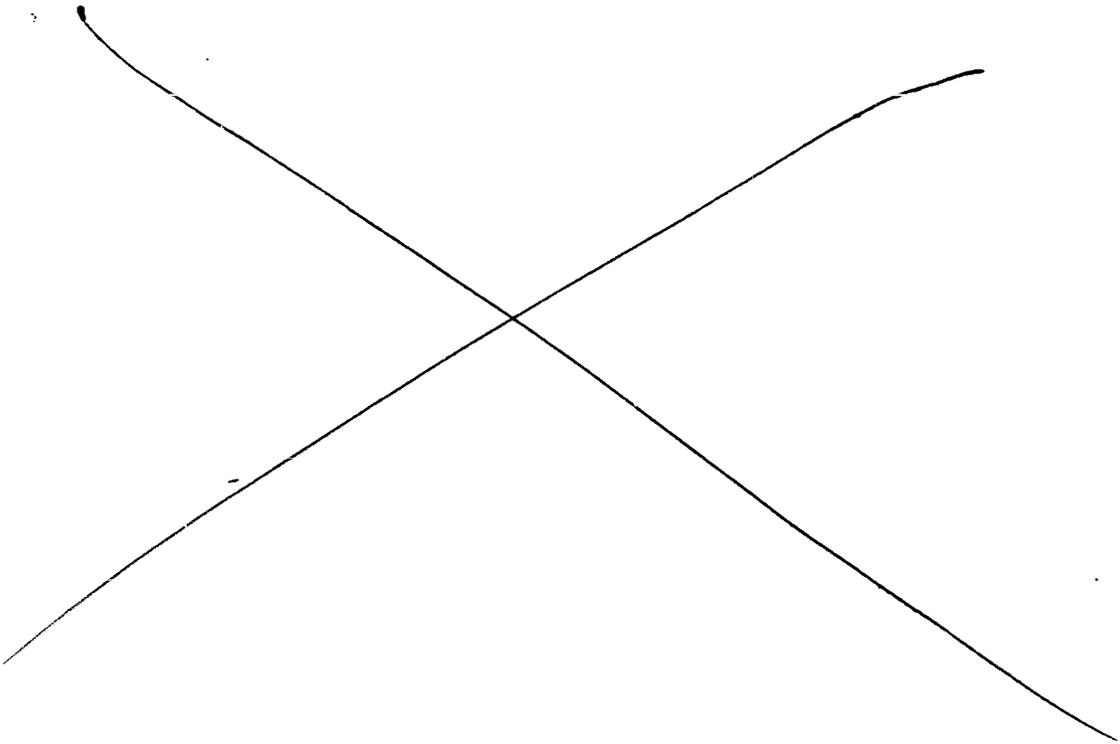
9/16/76

METHODOLOGY

Animals subjected to acute oral toxicity studies are fed by single-dose intubation using a calibrated syringe and a suitable rubber catheter. In the case of small rats or mice a blunt hypodermic needle is substituted for the catheter. Animals are fasted overnight prior to dosing. Materials are administered in the undiluted form or prepared as suspensions or solutions in water or corn oil. All animals are weighed and observed at intervals over a two-week post-feeding period or until any weight loss is regained and the animals appear healthy. Pathological observation is made on representative animals.

DATE

COMMENTS

- 9/2/76 Animals in cages 10 & 11 are lethargic, urine soaked, and have enlarged eyes.
- Remainder of animals - OK
- #02 in cage 11 gasping, blue in color, slight diarrhea and listless. Others OK at 2 hrs post dosage.
- 9/3/76 Animals in cages 9 & 10 are listless and have dark red eye secretions, Remainder - OK
- 

POW - TOXICOLOGY

REQUEST FOR PATHOLOGY

REQUESTED BY		CHARGE NUMBER		DATE 9/3/76
EAR MARK	SEX Male	SPECIES Rat	SAVE TISSUES <input type="checkbox"/> YES <input checked="" type="checkbox"/> NO	ROOM 49
MATERIAL N,N-Dimethylhydantoin				
DOSE CONCENTRATION Undiluted	NUMBER OF DOSES 1		ROUTE OF ADMINISTRATION	
DURATION OF DOSAGE	TIME SINCE LAST DOSE 24 hrs.		<input type="checkbox"/> DIETARY <input type="checkbox"/> INHALATION <input checked="" type="checkbox"/> ORAL <input type="checkbox"/> SKIN <input type="checkbox"/> METABOLISM <input type="checkbox"/> INJECTION (IP, IM, ETC.)	
CLINICAL SIGNS - (IF PRESENT)				

NECROPSY*	GROSS PATHOLOGY REPORT			PHOTOGRAPHED	DATE
	Cage	Comment	Time		
52-7	10 D	.316 g/kg			9-8-76 13-A
52-8	00C	.63			
52-9	11 B	1.26			
Dead → 52-10	01 A	2.52			

Animal A - dead

Ext. There is a very minimal amount of moistening of the hair in the region surrounding the prepuce. The abdomen appears to be somewhat distended on gross examination and Int. The urinary bladder is empty of urine. The GI tract- the large intestines from the cecum distally, contains some normal-appearing feces; however, the small intestines up to the point of the cecum is totally devoid of any normal ingesta and has a yellowish bile-colored fluid material within the lumen. The stomach is markedly distended with some feed and other material. Whether this is test material or not cannot be separated out. There is some hyperemia of the mucosal surface. No significant degree of hemorrhage or ulceration that I can recognize. Liver and kidneys are congested, but there are no other significant grossly recognizable changes.

Animal B

Externally NVL

Internally There is some normal-appearing ingesta and fecal material in the distal large intestines and distal part of the small intestines; however, the stomach again shows congestion and also the nonglandular portion of the squamous epithelium has sloughed from the mucosal surface, and in all probability, this may have been present in the previous animal; however, due to the large distension of the stomach with fluid and material, one did not readily see the mucosal surface as being admixed with the material. However, in view of the findings in this rat, in all probability, it also had occurred in that rat. Definite indications of gastric irritation, primarily in the area of squamous epithelial portion, were seen.

Animal C

Externally NVL

Internally The urinary bladder contains some normal urine. The large intestines contain normal fecal pellets; however, the small intestines in the proximal one-half contains more fluid-type material. The stomach is distended with fluid and the squamous epithelial

PATHOLOGIST (OVER)

*THE FOLLOWING TISSUES WERE EXAMINED AND UNLESS NOTED ABOVE NO VISIBLE LESIONS (NVL) WERE OBSERVED: TRACHEA, LUNG, HEART, LIVER, KIDNEYS, ADRENAL, SPLEEN, PANCREAS, STOMACH, SMALL INTESTINE, LARGE INTESTINE, AND REPRODUCTIVE ORGANS

MICROSCOPIC EXAMINATION*

DATE

portion of the stomach has submucosal edema such that the mucosa is separated from the rest of the wall of the stomach. The fundic portion of the stomach does not appear to show any significant gross change and no other internal viscera show anything of significant note.

Animal D

Ext. NVL

Int. The only significant finding is that there is still gastric edema within the nonglandular portion of the stomach and it has resulted in separation of the mucosal surface from the submucosal region.

At all dose levels, there are still changes within the gastric portion of the intestinal tract indicating a degree of irritation or certainly significant pathologic alterations despite the fact that the animals had lived, they were not without their local effects.

PATHOLOGIST

DATE

MIN GRADE:
COLOR:
ODOR:

ACCOUNT NO. _____ T NO. _____
CHANGE NO. _____ K NO. _____

N,N-Dimethylacetamide

657

MALE FEMALE

CASE NO. 200-4

CONCENTRATION 1 BY UNFILTERED

SOLVENT: WATER PROPYL OR ETHYL OTHER

COMMENTS	RESPONSE	NOT WASHED (LEFT)	WASHED (RIGHT)	DATE AND INITIALS
IMMEDIATE: 8:50	PAIN	2+	1	8/24/76
	CONJUNCTIVA	3	3	W
	CORNEA	1	3	
AFTER ONE HOUR (OR _____ HOURS)	CONJUNCTIVA	4+	4+	8/24/76
	BEFORE STAIN	3+	3+	W
	AFTER STAIN	2	4	
	INFORMED SUBJECTS IRITIS	2	2	
AFTER 24 HOURS	CONJUNCTIVA	5	4+	8/25/76
	BEFORE STAIN	3	3	W
	AFTER STAIN	3+	2	
	INFORMED SUBJECTS IRITIS	3	2	
AFTER 48 HOURS	CONJUNCTIVA	4+	4	8/26/76
	BEFORE STAIN	2+	2+	W
	AFTER STAIN	3	2	
	INFORMED SUBJECTS IRITIS	2	1	
AFTER 75 DAYS	CONJUNCTIVA	3	3	8/30/76
	BEFORE STAIN	1	1	W
	AFTER STAIN	1	1	6 days
	INFORMED SUBJECTS IRITIS	1	1	

a lot of hair is going from middle of back of eye.

DESCRIBE UNDER COMMENTS: _____
DATE: 9-8-76

EYE CONTACT TEST

Method:

Stain both eyes with fluorescein (5% in H_2O), wash promptly and examine for any evidence of injury. Allow rest period of 24 hours before introducing test material.

Introduce 2 drops of a liquid material, or a solution in the concentration called for (i. e. 100, 10, 1% etc.), onto the right eyeball. If a solid, use a small amount on a spatula. This eye is washed (within 30 sec.) for 2 minutes in a flowing stream of tepid water.

The left eye is then treated with 2 drops as described above, but the eye is left unwashed.

Both eyes are observed immediately for pain. Within 2 to 3 minutes after the unwashed eye is treated, each is observed for conjunctival and corneal response. Similar observations are made of both eyes at 1 hour, 24 hours, 48 hours and 6 to 8 days after treatment. Note that both eyes are stained with fluorescein (5% water sol'n.) at 1 hour, 24 hours, 48 hours, and 6 to 8 days. This necessitates the washing of both eyes to remove the excess stain.

Grading of Response:

A. Immediate Response (Pain)

1. No response
2. Very slight - No more than a few blinks - Normal in a minute or so.
3. Slight - blinks - tries to open but can't. Reflexes close eye.
4. Moderate. Holds eye shut and puts pressure on lids, may rub eye with paw.
5. Severe. Holds eye shut vigorously, rubs eye with paw - may squeal.
6. Very severe. Holds eye shut vigorously, May squeal, claws at eye, jumps, tries to escape.

B. Conjunctival Response

1. None
2. Very slight. Capillaries prominent. No swelling or general redness.
3. Slight. Conjunctival membranes somewhat inflamed. May be some sclero-corneal inflammation. Similar to response from a mild soap.
4. Moderate. Conjunctival membranes inflamed and sore, lids slightly swollen and reddened.
5. Severe. Conjunctival membranes red and swollen. Some pussy exudate; nictitating membrane sore and inflamed.
6. Very severe. Conjunctival membranes markedly reddened and swollen. Nictitating membrane edematous. Pussy exudate - eye may be stuck shut.

C. Corneal Response (Before staining)

1. No response.
2. Very slight. Questionable haziness.
3. Slight. Cloudy in part.
4. Moderate. Cloudy over whole but not opaque.
5. Severe. Cornea up to 50% opaque.
6. Very severe. Cornea completely opaque.

E. Internal Effects

1. No response.
2. Questionable.
3. Slight. Just perceptible.
4. Moderate. Definitely perceptible.
5. Severe. Marked change.
6. Very severe. Complete loss of function.

D. Corneal Response (After staining)

1. None
2. Very slight. Few diffuse areas of necrosis. Probably heal in 24-48 hours.
3. Slight. Up to 50% of eye covered with shallow necrosis. Probably heal O.K.
4. Moderate. 50-100% of eye necrotic but lesions are shallow. Doubtful if vision will be impaired.
5. Severe. Marked necrosis over whole area which may result in loss of eye.
6. Very severe. Eye lost. Heavy necrosis.

Comments:

Observations recorded in this space may include unusual types or severity of responses not fully covered by the descriptions under Grading of Response. Particular remarks may be made concerning the lids, nictitating membrane, iris, pupil, lens, or anterior chamber.

FORM GRADE _____
 BAR _____
 INTACT ABDOMEN _____
 ABRADED ABDOMEN _____

ACCOUNT NO. _____
 T. NO. _____
 CHARGE NO. _____

N,N-Dimethylacetamide

CASE NO. **309-1**

TEST BY REPEATED APPLICATION AS 10 MATERIAL SOLUTION IN:

DATE	8/12	8/24	8/29	8/26	8/27	8/30	9/7	9/13										
DAYS ON EXPOSURE	0	1	2	3	4	7	15	21										
ON EAR	1	2	3	4	5	6												
APPLICATION NO.	1	2	3	4	5	6												
HYPEREMIA		1	2	2+	3	3+	3+	3										
EDEMA		1	3+	3	4	4+	4	3										
NECROSIS		1	2	2	3	4	4	4										
EXFOLIATION		1	1	1	2	1	1	2										
HAIR LOSS		1	1	1	1	1	1	3										
SCAB		1	1	1	1	1	4	4										
SCAR		1	1	1	1	1	1	1										
THICKNESS (MM)		1	1	1	1	1	1	1										

ON ABDOMEN INTACT	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
APPLICATION NO.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
HYPEREMIA		4	4	4	4+	4	3	2										
EDEMA		3+	4	4	3+	3	3	3										
NECROSIS		1	2	3	4	4	5	3+										
EXFOLIATION		1	1	1	1	1	1	3										
SCAB		1	1	1	1	3+	5	4										
SCAR		1	1	1	1	1	1	1										
THICKNESS (MM)		1	1	1	1	1	1	1										

ON ABDOMEN ABRADED	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
APPLICATION NO.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
HYPEREMIA		1	4	4	4	4	3	2										
EDEMA		3+	4	4	3	3	3	3										
NECROSIS		1	2	4	4	4	5	3+										
EXFOLIATION		1	1	1	1	1	1	3										
SCAB		1	1	1	1	3+	5	4										
SCAR		1	1	1	1	1	1	1										

WEIGHT IN KG	404	404	404	404	404	359	350	346										
OBSERVATION BY	W	W	W	W	W	W	LL	W										

COMMENTS ON BACK OF THIS PAGE

SIGNED _____

DATE

9/13/76

METHODOLOGY

WHITE LABORATORY RABBITS ARE PREPARED FOR THIS TEST BY SHAVING THE HAIR FROM THE ENTIRE ABDOMEN WITH A STRAIGHT RAZOR AND BARBER SOAP. ANIMALS ARE THEN RESTED FOR SEVERAL DAYS TO ALLOW ANY ABRASIONS TO HEAL COMPLETELY AND TO BE SURE SKIN IS SUITABLE FOR USE. APPLICATIONS ARE MADE ACCORDING TO THE METHODS DESCRIBED BELOW AND REACTIONS AND OBSERVATIONS ARE RECORDED DAILY DURING THE APPLICATION PERIOD AND AT VARIOUS INTERVALS THEREAFTER. APPLICATIONS ARE USUALLY DISCONTINUED UPON PRODUCTION OF A SUBSTANTIAL SKIN BURN.

METHOD A (EAR)

LIQUIDS AND PASTES (NO SOLIDS) ARE APPLIED TO THE EAR. TEN APPLICATIONS ARE MADE OVER A PERIOD OF 14 DAYS.

METHOD B (INTACT ABDOMEN)

LIQUIDS AND SOLIDS ARE APPLIED UNDER A 1 INCH BY 1 INCH COTTON PAD AND HELD IN PLACE BY A CLOTH BANDAGE TAPED TO THE HAIR. TEN APPLICATIONS ARE MADE OVER A PERIOD OF 14 DAYS. THIS ALLOWS CONTINUOUS, INTIMATE, CONTACT WITH THE SKIN FOR A 2 WEEK PERIOD.

METHOD C (ABRADED ABDOMEN)

A 1 INCH BY 1 INCH AREA OF SKIN ABOUT 1 INCH BY 1 INCH IS CROSS-HATCHED WITH A SHARP HYPODERMIC NEEDLE TO PENETRATE THE STRATUM CORNEUM BUT NOT TO PRODUCE MORE THAN A TRACE OF BLEEDING. LIQUIDS AND SOLIDS ARE APPLIED AS IN METHOD B. THREE CONSECUTIVE DAILY APPLICATIONS ONLY ARE MADE WHICH ALLOWS FOR 3 DAYS OF INTIMATE, CONFINED, CONTACT WITH THE ABRADED SKIN.

GRADE	PEREMIA	EDEMA	NECROSIS	EXFOLIATION	HAIR LOSS	SCAB	SCAR
1	NONE	NONE	NONE	NONE	NONE	NONE	NONE
2	QUESTIONABLE	QUESTIONABLE	QUESTIONABLE	QUESTIONABLE	QUESTIONABLE	QUESTIONABLE	QUESTIONABLE
3	SLIGHT PINK	SLIGHT	SUPERFICIAL	SLIGHT	SLIGHT	SLIGHT CRUSTATION	SLIGHT
4	MODERATE PINK	MODERATE	MODERATE	MODERATE	MODERATE	MODERATE CRUSTATION	MODERATE
5	RED	MARKED	DEEP	MARKED	MARKED	MARKED SCAB	MARKED
6	VERY RED	SEVERE	VERY DEEP	SEVERE	SEVERE	DEEP SCAB	SEVERE

DATE:

COMMENTS:

8/24 Areas below and above application sites are swollen (moderate).

8/25 A great deal of edema is visible in areas approximately 2 inches below or above the application sites. The bandage was removed for 1-2 hours prior to the third application of material. At the end of this period the swelling moved from the area indicated on the diagram to the center of the animal's abdomen. The edema had also subsided.

8/26 Edema has greatly subsided in areas other than application sites.

9/7 The entire shaved area is covered with scab & necrosis. There is pus under the scab in places. The necrosis has extended to the thighs & the sides of the animal and is very severe. In all these areas, though there is little redness or edema apparent at this time. 9/13 - Same

ETHANAMINE, N,N-DIETHYL-, (Synonym: TRIETHYLAMINE)
CAS# 121-44-8

This substance is not manufactured or imported by Dow. We purchase it from Pennwalt, Union Carbide, and in the past have bought it from Air Products and Chemicals. A Pennwalt MSDS is enclosed.

Triethylamine is used by Dow in small amounts in several different processes, and is used to make an amine salt of a herbicide product. It is a raw material in 133 Dow Products, and is present as an impurity in approximately 18 Products. MSD sheets for 3 products in which it is present in small amounts are enclosed.

An environmental study on predicting the flux of organics across the air/water interface, which included triethylamine as one of the organics studied, was found in our files. A copy is enclosed.

A sheet of summary environmental data is also enclosed.

J.W. Turley
10-3-88

SUMMARY ENVIRONMENTAL DATA FOR
SELECTED TSCA SECTION 8(D) OR ITC LISTED SUBSTANCES

PAGE 1
05/02/88

THIS SUMMARY INCLUDES IDENTIFYING NUMBERS AND NAMES, AND DATA ON
ENVIRONMENTAL DISTRIBUTION, FATE, AND TOXICITY FOR SPECIFIC SUBSTANCES LISTED

THIS PAGE CONTAINS DATA FOR: CAS# = 121-44-8
ETHANAMINE: N,N-DIETHYL-
TRIETHYLAMINE

AER	BOD5	BOD10	BOD20	BOD28	COD	THOD	FHMNOEL	FHMLC50	DMLC50
15	0.00	0.00	0.00		0.91	3.49	30	44.7	34

ABBREVIATIONS: AER - AERATION FROM WATER IN 4 HOURS, %
BOD - BIOCHEMICAL OXYGEN DEMAND, PARTS/PART BY WT
COD - CHEMICAL OXYGEN DEMAND, PARTS/PART BY WT
THOD - THEORETICAL OXYGEN DEMAND, PARTS/PART BY WT
FHM - FATHEAD MINNOW
DM - DAPHNIA MAGNA
NOEL - NO OBSERVED EFFECT LEVEL, MG/L
LC50 - LETHAL CONCENTRATION, 50% MORTALITY, MG/L

MATERIAL SAFETY DATA SHEET

Recd. 11-16-87

PENNWALT CORPORATION
ORGANIC CHEMICALS
THREE PARKWAY
PHILADELPHIA, PA 19102

EMERGENCY PHONE NUMBERS
BUSINESS HOURS : 215-587-7707
OTHER TIMES : 313-285-9200

PRODUCT IDENTIFICATION

PRODUCT NAME: TRIETHYLAMINE
CAS NO.: 121-44-9
CHEMICAL NAME: ETHANAMINE, N,N-DIETHYL
MOLECULAR FORMULA: C6H15N
SYNONYMS: NA
CHEMICAL FAMILY: ALKYL AMINE

INGREDIENTS---HAZARD CLASSIFICATIONS

COMPONENTS:	CAS NO.:	% OSHA:	NFPA:
TRIETHYLAMINE	121-44-8	99 FLAMMABLE CORROSIVE TOXIC	2-3-0

SHIPPING INFORMATION

T: RQ TRIETHYLAMINE; FLAMMABLE LIQUID; UN 1296; FLAMMABLE PLACARDS.
DUMPER & DRUMS: TRIETHYLAMINE; FLAMMABLE LIQUID; UN 1296; CHEMICALS
NOISE.
TC: RQ TRIETHYLAMINE; FLAMMABLE LIQUID; UN 1296; PLACARDED FLAMMABLE.

PHYSICAL PROPERTIES

BOILING POINT/RANGE: 85-91 C 185-196 F	MELTING POINT: -115 C -175 F	FREEZING POINT: NA
MOLECULAR WEIGHT: 101.2	SPECIFIC GRAVITY(H2O=1): .726-.730 @ 20/20 C	VAPOR PRESSURE(4MM HG): 52 @ 20 C 68 F
VAPOR DENSITY(AIR=1): 3.5	SOLUBILITY IN H2O: 10% @ 20C, 2% @ 60 C	% VOLATILES BY VOLUME: 100

APPEARANCE AND ODOR:
WATER WHITE LIQUID. AMINE ODOR.

NA - NOT APPLICABLE NE - NOT ESTABLISHED
) - INDICATES REGISTERED TRADEMARK OF PENNWALT CORPORATION

TOXICITY - CONTINUED

TOXICITY COMMENTS:

CHRONIC: RATS GIVEN MORE THAN 200 PPM OF TRIETHYLAMINE IN DRINKING WATER FOR MULTIPLE GENERATIONS REPORTEDLY SHOWED NO EFFECTS.

HEALTH HAZARD INFORMATION

PERMISSIBLE EXPOSURE LIMITS:

ACGIH 1983 10 PPM / OSHA 1983 TWA 10 PPM, 40 MG/M3
OTHER: STEL: 15 PPM, 60 MG/M3.

EMERGENCY FIRST AID

INGESTION:

DO NOT INDUCE VOMITING GIVE PLENTY OF WATER GET MEDICAL ATTENTION

NEVER GIVE ANYTHING BY MOUTH TO AN UNCONSCIOUS PERSON.

DERMAL:

WASH WITH SOAP AND WATER GET MEDICAL ATTENTION CONTAMINATED CLOTHING - REMOVE AND LAUNDR CONTAMINATED SHOES - DESTROY

EYE CONTACT:

FLUSH WITH PLENTY OF WATER FOR AT LEAST 15 MINUTES GET MEDICAL ATTENTION

INHALATION:

REMOVE TO FRESH AIR IF NOT BREATHING GIVE ARTIFICIAL RESPIRATION GIVE OXYGEN GET MEDICAL ATTENTION

SPECIAL PROTECTION INFORMATION

VENTILATION REQUIREMENTS:

USE WITH ADEQUATE VENTILATION

EYE:

FACE SHIELD GOGGLES

HAND(GLOVE TYPE):

SYNTHETIC RUBBER ANY NON-PERMEABLE GLOVE

RESPIRATOR TYPE:

SELF-CONTAINED SUPPLIED AIR

RESPIRATORS FOR ENTERING ENCLOSED AREA CONTAINING SPILL OR FIRE.

NA - NOT APPLICABLE NE - NOT ESTABLISHED
) - INDICATES REGISTERED TRADEMARK OF PENNWALT CORPORATION

SPECIAL PROTECTION INFORMATION - CONTINUED

OTHER PROTECTIVE EQUIPMENT: RUBBER BOOTS APRON

SPECIAL HANDLING AND STORAGE CONDITIONS

WASH THOROUGHLY AFTER HANDLING

DO NOT GET IN EYES, ON SKIN OR CLOTHING

DO NOT BREATHE DUST, VAPOR, MIST, GAS

KEEP CONTAINER CLOSED

KEEP AWAY FROM HEAT, SPARKS, AND OPEN FLAMES

USE EXPLOSION PROOF EQUIPMENT

EMPTY CONTAINER MAY CONTAIN HAZARDOUS RESIDUES

SPILL MANAGEMENT

ABSORBS WITH SAND OR INERT MATERIAL

PREVENT SPREAD OF SPILL

FOR SMALL SPILLS (LESS THAN 5 GALS.) FLUSH AREA WITH WATER. LARGE SPILLS: DIKE TO PREVENT SPREAD. REMOVE TO CLOSED CONTAINER. THEN, RINSE SPILL AREA WITH WATER.

DISPOSAL PROCEDURES

CONSULT FEDERAL, STATE, OR LOCAL AUTHORITIES FOR PROPER DISPOSAL PROCEDURES.

MSDS PREPARED BY LEE W. DIESTELOW

THE ABOVE INFORMATION IS ACCURATE TO THE BEST OF OUR KNOWLEDGE. HOWEVER, SINCE DATA, SAFETY STANDARDS, AND GOVERNMENT REGULATIONS ARE SUBJECT TO CHANGE AND THE CONDITIONS OF HANDLING AND USE, OR MISUSE ARE BEYOND OUR CONTROL, PENNWALT MAKES NO WARRANTY, EITHER EXPRESS OR IMPLIED, WITH RESPECT TO THE COMPLETENESS OR CONTINUING ACCURACY OF THE INFORMATION CONTAINED HEREIN AND DISCLAIMS ALL LIABILITY FOR RELIANCE THEREON. USER SHOULD SATISFY HIMSELF THAT HE HAS ALL CURRENT DATA RELEVANT TO HIS PARTICULAR USE.

NA - NOT APPLICABLE NE - NOT ESTABLISHED) - INDICATES REGISTERED TRADEMARK OF PENNWALT CORPORATION

MATERIAL SAFETY DATA SHEET

Dow Chemical U.S.A.* Midland, MI 48674 Emergency Phone: 517-636-4400

Product Code: 03093

Page: 1

PRODUCT NAME: CPR (R) 477B-2.2 RIGID SYSTEM

Effective Date: 03/20/88 Date Printed: 04/12/88

MSD: 002362

1. INGREDIENTS:

Trichlorofluoromethane (Fluorocarbon)	CAS# 000075-69-4	13%
Blend of polyether polyols	CAS# 009088-00-2	
	CAS# 068609-24-5	
	CAS# 025791-96-2	
Water	CAS# 007732-18-5	

This document is prepared pursuant to the OSHA Hazard Communication Standard (29 CFR 1910.1200). In addition, other substances not 'Hazardous' per this OSHA Standard may be listed. Where proprietary ingredient shows, the identity may be made available as provided in this standard.

2. PHYSICAL DATA:

BOILING POINT: 74.5F (23.6C) - (fluorocarbon 11)
VAP. PRESS: 798 mmHg @ 25C (fluorocarbon 11)
VAP. DENSITY: Not determined
SOL. IN WATER: Slight
SP. GRAVITY: 1.2
APPEARANCE: Brownish liquid.
ODOR: Sweetish, faint amine odor.

CAS 121-44-8

15 in this

at 0.6% max

usually ~ 0.5%

3. FIRE AND EXPLOSION HAZARD DATA:

FLASH POINT: 350F, 177C
METHOD USED: COC

FLAMMABLE LIMITS

LFL: Not determined
UFL: Not determined

URETHANES UNLIMITED

EXTINGUISHING MEDIA: Water fog, foam, CO2, and dry chemical.

FIRE AND EXPLOSION HAZARDS: Will not burn until fluorocarbon boils away. Contains volatile blowing agent (fluorocarbon 11). Excessive heat can cause dangerous pressure buildup in closed containers. Thermal decomposition of fluorocarbon 11 in air can generate toxic phosgene.

FIRE-FIGHTING EQUIPMENT: Wear positive pressure self-contained breathing apparatus.

4. REACTIVITY DATA:

STABILITY: (CONDITIONS TO AVOID) Stable under recommended

(Continued on Page 2)

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MATERIAL SAFETY DATA SHEET

Dow Chemical U.S.A.* Midland, MI 48674 Emergency Phone: 517-636-4400

PRODUCT NAME: CPR (R) 477B-2.2 RIGID SYSTEM Product Code: 03093 Page: 2

Effective Date: 03/20/88 Date Printed: 04/12/88 MSD: 002362

4. REACTIVITY DATA: (CONTINUED)

storage conditions. Store in original, unopened container at 65-85F. Excessive heat above the boiling point of fluorocarbon can cause dangerous pressure buildup in closed containers.

INCOMPATIBILITY: (SPECIFIC MATERIALS TO AVOID) Strong oxidizers, strong acids, and alkali or alkaline earth metals (copper, zinc, brass).

HAZARDOUS DECOMPOSITION PRODUCTS: Carbon monoxide, carbon dioxide, traces of nitrogen oxides, phosgene, and hydrogen cyanide.

HAZARDOUS POLYMERIZATION: Will not occur.

5. ENVIRONMENTAL AND DISPOSAL INFORMATION:

ACTION TO TAKE FOR SPILLS: Spills should be contained to prevent contamination of waterways. Dike spill and cover with oil absorbent material and sweep up.

DISPOSAL METHOD: Incinerate or bury in an approved landfill in accordance with local, state, and federal regulations.

6. HEALTH HAZARD DATA:

EYE: May cause slight eye irritation. Corneal injury is unlikely.

SKIN CONTACT: Prolonged or repeated exposure not likely to cause significant skin irritation.

SKIN ABSORPTION: A single prolonged exposure is not likely to result in the material being absorbed through skin in harmful amounts. The LD50 for skin absorption in rabbits is >2000 mg/kg.

INGESTION: Single dose oral toxicity is low. The oral LD50 for rats is >4000 mg/kg.

INHALATION: Component trichlorofluoromethane is volatile at room temperature. In man, exposure to concentrations > 2500 ppm may cause central nervous system, anesthetic or narcotic effects; at levels > 5000 ppm, it may increase sensitivity to epinephrine and increase irregular heartbeats. Vapors are unlikely from the polyol components at room temperatures; elevated temperatures may generate vapor levels

(Continued on Page 3)

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MATERIAL SAFETY DATA SHEET

Dow Chemical U.S.A.* Midland, MI 48674 Emergency Phone: 517-636-4400

Product Code: 03093

Page: 3

PRODUCT NAME: CPR (R) 477B-2.2 RIGID SYSTEM

Effective Date: 03/20/88 Date Printed: 04/12/88

MSD: 002362

6. HEALTH HAZARD DATA: (CONTINUED)

sufficient to cause irritation.

SYSTEMIC & OTHER EFFECTS: Based on available data, repeated exposures to the polyol and trichlorofluoromethane components are not expected to cause additional significant adverse effects. Component trichlorofluoromethane did not cause cancer in laboratory animals in long-term animal studies. Results of in vitro (test tube) mutagenicity tests on component trichlorofluoromethane were negative.

7. FIRST AID:

EYES: Irrigate immediately with water for at least 5 minutes.

SKIN: Wash off in flowing water or shower.

INGESTION: Induce vomiting if large amounts are ingested. Consult medical personnel.

INHALATION: Remove to fresh air. If not breathing, give mouth-to-mouth resuscitation. If breathing is difficult, give oxygen. Call a physician.

NOTE TO PHYSICIAN: Exposure may increase "myocardial irritability." Do not administer sympathomimetic drugs unless absolutely necessary. No specific antidote. Supportive care. Treatment based on judgment of the physician in response to reactions of the patient.

8. HANDLING PRECAUTIONS:

EXPOSURE GUIDELINE(S): ACGIH TLV (ceiling) and OSHA PEL is 1000 ppm for trichlorofluoromethane.

VENTILATION: Provide general and/or local exhaust ventilation to control airborne levels below the exposure guidelines.

RESPIRATORY PROTECTION: Atmospheric levels should be maintained below the exposure guideline. When respiratory protection is required for certain operations, use an approved air-purifying respirator. For emergency and other conditions where the exposure guideline may be greatly exceeded, use an approved positive pressure self-contained breathing apparatus.

SKIN PROTECTION: For brief contact, no precautions other than

(Continued on Page 4)

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M A T E R I A L S A F E T Y D A T A S H E E T

Dow Chemical U.S.A.* Midland, MI 48674 Emergency Phone: 517-636-4400

Product Code: 03093 Page: 4
PRODUCT NAME: CPR (R) 477B-2.2 RIGID SYSTEM

Effective Date: 03/20/88 Date Printed: 04/12/88 MSD: 002362

8. HANDLING PRECAUTIONS: (CONTINUED)

clean body-covering clothing should be needed. When prolonged or frequently repeated contact could occur, use protective clothing impervious to this material. Selection of specific items such as gloves, boots, apron or full-body suit will depend on operation.

EYE PROTECTION: Use safety glasses. Where contact with liquid is likely, chemical goggles are recommended because eye contact with this material may cause pain, even though it is unlikely to cause injury.

9. ADDITIONAL INFORMATION:

REGULATORY REQUIREMENTS:

SARA HAZARD CATEGORY: This product has been reviewed according to the EPA 'Hazard Categories' promulgated under Sections 311 and 312 of the Superfund Amendment and Reauthorization Act of 1986 (SARA Title III) and is considered, under applicable definitions, to meet the following categories:

An immediate health hazard
A delayed health hazard

SPECIAL PRECAUTIONS TO BE TAKEN IN HANDLING AND STORAGE: Store in original, unopened containers at 65-85F. Replace outage with dry, inert atmosphere. Cautiously vent pressure buildup prior to fully opening container.

Do not store or handle this material in alkali or alkaline earth metals or metals of construction, and in particular, copper and zinc, as well as the alloy brass.

MSDS STATUS: Revised Section 9.

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The Information Herein Is Given In Good Faith, But No Warranty,
Express Or Implied, Is Made. Consult The Dow Chemical Company
For Further Information.

MATERIAL SAFETY DATA SHEET

Dow Chemical U.S.A.* Midland, MI 48674 Emergency Phone: 517-636-4400

Product Code: 03089

Page: 1

PRODUCT NAME: CPR (R) 461B RIGID SYSTEM

Effective Date: 03/20/88 Date Printed: 04/12/88

MSD: 002548

1. INGREDIENTS:

Trichlorofluoromethane (F11)	CAS# 000075-69-4	10%
Triethylamine	CAS# 000121-44-8	2%
Blend of polyether polyols	CAS# 0257	
	CAS# 0372	
Organophosphate flame retardant	CAS# 0027	
Silicone surfactant		

This document is prepared pursuant to the OSHA Communication Standard (29 CFR 1910.1200). In substances not 'Hazardous' per this OSHA Standard where proprietary ingredient shows, the identity available as provided in this standard.

*Normally 1.6%
or less
but it is present*

2. PHYSICAL DATA:

BOILING POINT: 74.5F (23.6C) (F11)
VAP. PRESS: 798 mmHg @ 25C (F11)
VAP. DENSITY: Not determined
SOL. IN WATER: Nil
SP. GRAVITY: >1
APPEARANCE: Brownish liquid.
ODOR: Sweetish amine odor.

URETHANES UNLIMITED

3. FIRE AND EXPLOSION HAZARD DATA:

FLASH POINT: >350 F, >177C
METHOD USED: COC; ASTM - D92

FLAMMABLE LIMITS

LFL: Not determined
UFL: Not determined

EXTINGUISHING MEDIA: Water fog, foam, CO2, and dry chemical.

FIRE AND EXPLOSION HAZARDS: Will not burn until fluorocarbon boils away. Contains volatile blowing agent (F11). Excessive heat can cause dangerous pressure build-up in closed containers. Thermal decomposition of F11 in air can generate toxic phosgene.

FIRE-FIGHTING EQUIPMENT: Wear positive pressure self-contained breathing apparatus.

(Continued on Page 2)

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MATERIAL SAFETY DATA SHEET

Dow Chemical U.S.A.* Midland, MI 48674 Emergency Phone: 517-636-4400

Product Code: 03089 Page: 2
PRODUCT NAME: CPR (R) 461B RIGID SYSTEM

Effective Date: 03/20/88 Date Printed: 04/12/88 MSD: 002548

4. REACTIVITY DATA:

STABILITY: (CONDITIONS TO AVOID) Excessive heat above the boiling point of fluorocarbon can cause dangerous pressure build-up in closed containers. Stable at recommended storage conditions. Store in original, unopened containers at 65-85F.

INCOMPATIBILITY: (SPECIFIC MATERIALS TO AVOID) Strong oxidizers, strong acids, and alkali or alkaline earth metals (copper, zinc, brass).

HAZARDOUS DECOMPOSITION PRODUCTS: Carbon monoxide, carbon dioxide, traces of nitrogen oxides, phosgene, and hydrogen cyanide under fire conditions.

HAZARDOUS POLYMERIZATION: Will not occur.

5. ENVIRONMENTAL AND DISPOSAL INFORMATION:

ACTION TO TAKE FOR SPILLS: Spills should be contained to prevent contamination of waterways. Dike spill and cover with oil absorbent material and sweep up.

DISPOSAL METHOD: Incinerate or bury in an approved landfill in accordance with local, state, and federal regulations.

6. HEALTH HAZARD DATA:

EYE: May cause slight eye irritation.

SKIN CONTACT: Prolonged or repeated exposure may cause skin irritation. May cause allergic skin reaction in susceptible individuals.

SKIN ABSORPTION: A single prolonged exposure is not likely to result in the material being absorbed through skin in harmful amounts. The dermal LD50 has not been determined.

INGESTION: Single dose oral toxicity is believed to be low. Single dose oral LD50 has not been determined.

INHALATION: Component trichlorofluoromethane is volatile at room temperature. In man, exposure to concentrations > 2500 ppm may cause central nervous system, anesthetic or narcotic effects; at levels > 5000 ppm, it may increase sensitivity to epinephrine and increase irregular heartbeats. Vapors or mists of polyol and flame retardant components may cause eye and

(Continued on Page 3)

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MATERIAL SAFETY DATA SHEET

Dow Chemical U.S.A.* Midland, MI 48674 Emergency Phone: 517-636-4400

Product Code: 03089

Page: 3

PRODUCT NAME: CPR (R) 461B RIGID SYSTEM

Effective Date: 03/20/88

Date Printed: 04/12/88

MSD: 002548

6. HEALTH HAZARD DATA: (CONTINUED)

respiratory irritation and/or central nervous system depression, especially if the material is heated.

SYSTEMIC & OTHER EFFECTS: Repeated excessive exposure to the flame retardant may cause liver and kidney effects. Component trichlorofluoromethane did not cause cancer in laboratory animals in long-term animal studies. In vitro (test tube) mutagenicity studies on component trichlorofluoromethane were negative.

7. FIRST AID:

EYES: Irrigate immediately with water for at least 5 minutes.

SKIN: Wash off in flowing water or shower.

INGESTION: Induce vomiting if large amounts are ingested. Consult medical personnel.

INHALATION: Remove to fresh air. If not breathing, give mouth-to-mouth resuscitation. If breathing is difficult, give oxygen. Call a physician.

NOTE TO PHYSICIAN: Exposure may increase "myocardial irritability." Do not administer sympathomimetic drugs unless absolutely necessary. No specific antidote. Supportive care. Treatment based on judgment of the physician in response to reactions of the patient.

8. HANDLING PRECAUTIONS:

EXPOSURE GUIDELINE(S): OSHA PEL is 1000 ppm for fluorotrichloromethane. ACGIH TLV is 1000 ppm ceiling for trichlorofluoromethane.

VENTILATION: Provide general and/or local exhaust ventilation to control airborne levels below the exposure guidelines.

RESPIRATORY PROTECTION: Atmospheric levels should be maintained below the exposure guideline. When respiratory protection is required for certain operations, use an approved air-purifying respirator. If respiratory irritation is experienced, use an approved air-purifying respirator. For emergency and other conditions where the exposure guideline may be greatly exceeded, use an approved positive pressure self-contained breathing

(Continued on Page 4)

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MATERIAL SAFETY DATA SHEET

Dow Chemical U.S.A.* Midland, MI 48674 Emergency Phone: 517-636-4400

Product Code: 03089

Page: 4

PRODUCT NAME: CPR (R) 461B RIGID SYSTEM

Effective Date: 03/20/88 Date Printed: 04/12/88

MSD: 002548

8. HANDLING PRECAUTIONS: (CONTINUED)

apparatus.

SKIN PROTECTION: For brief contact, no precautions other than clean body-covering clothing should be needed. When prolonged or frequently repeated contact could occur, use protective clothing impervious to this material. Selection of specific items such as gloves, boots, apron or full-body suit will depend on operation.

EYE PROTECTION: Use safety glasses. Where contact with this material is likely, chemical goggles are recommended because eye contact may cause pain even though it is unlikely to cause injury.

9. ADDITIONAL INFORMATION:

REGULATORY REQUIREMENTS:

SARA HAZARD CATEGORY: This product has been reviewed according to the EPA 'Hazard Categories' promulgated under Sections 311 and 312 of the Superfund Amendment and Reauthorization Act of 1986 (SARA Title III) and is considered, under applicable definitions, to meet the following categories:

A delayed health hazard
A reactive hazard

SPECIAL PRECAUTIONS TO BE TAKEN IN HANDLING AND STORAGE: Store in original, unopened containers at 65-85F. Replace outage with dry, inert atmosphere. Cautiously vent pressure buildup prior to fully opening container. Contains Flammable - protect from excessive heat.

Do not store or handle this material in alkali or alkaline earth metals or metals of construction, and in particular copper and zinc, as well as the alloy brass.

MSDS STATUS: Revised Section 9.

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MATERIAL SAFETY DATA SHEET

Dow Chemical U.S.A.* Midland, MI 48674 Emergency Phone: 517-636-4400

Product Code: 03091

Page: 1

PRODUCT NAME: CPR (R) 477B-1.8 RIGID SYSTEM

Effective Date: 03/20/88

Date Printed: 04/12/88

MSD: 002363

1. INGREDIENTS:

Trichlorofluoromethane (Fluorocarbon 11)	CAS# 000075-69-4	18%
Polyether polyol blend	CAS# 009082-00-2, 068609-24-5, 025791-96-2	
Water	CAS# 007732-18-5	

This document is prepared pursuant to the OSHA Hazard Communication Standard (29 CFR 1910.1200). In addition, other substances not 'Hazardous' per this OSHA Standard may be listed. Where proprietary ingredient shows, the identity may be made available as provided in this standard.

2. PHYSICAL DATA:

BOILING POINT: 74.5F (23.6C) - (Fluorocarbon 11)
VAP. PRESS: 798 mmHg @ 25C (Fluorocarbon 11)
VAP. DENSITY: Not determined
SOL. IN WATER: Slight
SP. GRAVITY: 1.2
APPEARANCE: Brownish liquid.
ODOR: Sweetish, faint amine odor.

*CAS 121-44-8
is in this way
of 0.7% and
normally = 0.6%*

3. FIRE AND EXPLOSION HAZARD DATA:

FLASH POINT: 350F, 177C
METHOD USED: COC

FLAMMABLE LIMITS
LFL: Not determined
UFL: Not determined

URETHANES UNLIMITED

EXTINGUISHING MEDIA: Water fog, foam, CO2, and dry chemical.

FIRE AND EXPLOSION HAZARDS: Will not burn until fluorocarbon boils away. Contains volative blowing agent (Fluorocarbon 11). Excessive heat can cause dangerous pressure buildup in closed containers. Thermal decomposition of Fluorocarbon 11 in air can generate toxic phosgene.

FIRE-FIGHTING EQUIPMENT: Wear positive pressure self-contained breathing apparatus.

4. REACTIVITY DATA:

STABILITY: (CONDITIONS TO AVOID) Excessive heat above the

(Continued on Page 2)

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MATERIAL SAFETY DATA SHEET

Dow Chemical U.S.A.* Midland, MI 48674 Emergency Phone: 517-636-4400

Product Code: 03091 Page: 2
PRODUCT NAME: CPR (R) 477B-1.8 RIGID SYSTEM

Effective Date: 03/20/88 Date Printed: 04/12/88 MSD: 002363

4. REACTIVITY DATA: (CONTINUED)

boiling point of fluorocarbon can cause dangerous pressure buildup in closed containers. Stable under recommended storage conditions. Store in original, unopened container at 65-85F.

INCOMPATIBILITY: (SPECIFIC MATERIALS TO AVOID) Strong oxidizers, strong acids, and alkali or alkaline earth metals (copper, zinc, brass).

HAZARDOUS DECOMPOSITION PRODUCTS: Carbon monoxide, carbon dioxide, traces of nitrogen oxides, phosgene, and hydrogen cyanide.

HAZARDOUS POLYMERIZATION: Will not occur.

5. ENVIRONMENTAL AND DISPOSAL INFORMATION:

ACTION TO TAKE FOR SPILLS: Spills should be contained to prevent contamination of waterways. Dike spill and cover with oil absorbent material and sweep up.

DISPOSAL METHOD: Incinerate or bury in an approved landfill in accordance with local, state, and federal regulations.

6. HEALTH HAZARD DATA:

EYE: May cause slight eye irritation and slight corneal injury.

SKIN CONTACT: Prolonged exposure not likely to cause significant skin irritation. Repeated exposure may cause skin irritation.

SKIN ABSORPTION: A single prolonged exposure is not likely to result in the material being absorbed through skin in harmful amounts. The dermal LD50 has not been determined.

INGESTION: Single dose oral toxicity is believed to be low. Single dose oral LD50 has not been determined.

INHALATION: The Fluorocarbon 11 component in this mixture is volatile at room temperature. In man, exposure to concentrations of Fluorocarbon 11 > 2500 ppm may cause central nervous system, anesthetic or narcotic effects; at levels > 500 ppm, it may increase sensitivity to epinephrine and increase irregular heartbeats. Vapors are unlikely from the polyol components at room temperatures; elevated temperatures may generate vapor

(Continued on Page 3)

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M A T E R I A L S A F E T Y D A T A S H E E T

Dow Chemical U.S.A.* Midland, MI 48674 Emergency Phone: 517-636-4400

PRODUCT NAME: CPR (R) 477B-1.8 RIGID SYSTEM Product Code: 03091 Page: 3

Effective Date: 03/20/88 Date Printed: 04/12/88 MSD: 002363

6. HEALTH HAZARD DATA: (CONTINUED)

levels sufficient to cause irritation.

SYSTEMIC & OTHER EFFECTS: Based on available data, repeated exposures to the polyol and trichlorofluoromethane components are not expected to cause additional significant adverse effects. Component trichlorofluoromethane did not cause cancer in laboratory animals in long-term animal studies. Results of in vitro (test tube) mutagenicity tests on component trichlorofluoromethane were negative.

7. FIRST AID:

EYES: Irrigate immediately with water for at least 5 minutes.

SKIN: Wash off in flowing water or shower.

INGESTION: Induce vomiting if large amounts are ingested. Consult medical personnel.

INHALATION: Remove to fresh air. If not breathing, give mouth-to-mouth resuscitation. If breathing is difficult, give oxygen. Call a physician.

NOTE TO PHYSICIAN: Exposure may increase "myocardial irritability." Do not administer sympathomimetic drugs unless absolutely necessary. No specific antidote. Supportive care. Treatment based on judgment of the physician in response to reactions of the patient.

8. HANDLING PRECAUTIONS:

EXPOSURE GUIDELINE(S): ACGIH TLV (ceiling) and OSHA PEL is 1000 ppm for trichlorofluoromethane.

VENTILATION: Provide general and/or local exhaust ventilation to control airborne levels below the exposure guidelines.

RESPIRATORY PROTECTION: Atmospheric levels should be maintained below the exposure guideline. When respiratory protection is required for certain operations, use an approved air-purifying respirator. For emergency and other conditions where the exposure guideline may be greatly exceeded, use an approved positive pressure self-contained breathing apparatus.

SKIN PROTECTION: For brief contact, no precautions other than

(Continued on Page 4)

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M A T E R I A L S A F E T Y D A T A S H E E T

Dow Chemical U.S.A.* Midland, MI 48674 Emergency Phone: 517-636-4400

Product Code: 03091 Page: 4
PRODUCT NAME: CPR (R) 477B-1.8 RIGID SYSTEM

Effective Date: 03/20/88 Date Printed: 04/12/88 MSD: 002363

8. HANDLING PRECAUTIONS: (CONTINUED)

clean body-covering clothing should be needed. When prolonged or frequently repeated contact could occur, use protective clothing impervious to this material. Selection of specific items such as gloves, boots, apron or full-body suit will depend on operation.

EYE PROTECTION: Use chemical goggles.

9. ADDITIONAL INFORMATION:

REGULATORY REQUIREMENTS:

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An immediate health hazard
A delayed health hazard

SPECIAL PRECAUTIONS TO BE TAKEN IN HANDLING AND STORAGE: Store in original, unopened containers at 65-85F. Replace outage with dry, inert atmosphere. Cautiously vent pressure buildup prior to fully opening container.

Do not store or handle this material in alkali or alkaline earth metals or metals of construction, and in particular, copper and zinc, as well as the alloy brass.

MSDS STATUS: Revised Section 9.

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R & D REPORT

DOW CHEMICAL U.S.A.

CRI NUMBER	
LABORATORY REPORT CODE	
DATE ISSUED August 19, 1975	
LAB. NO.	PROBLEM NO.

DEPARTMENT Environmental Sciences Research

TITLE Predicting the Flux of Organics Across the Air Water Interface (Note: This Report contains information on Ethanamine, N,N-Diethyl-, CAS No. 121-44-8)	PAGES IN FULL REPORT 15
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AUTHOR(S)

REVIEWER'S SIGNATURE

This report is:	<input type="checkbox"/> INTERIM	and mainly:	<input checked="" type="checkbox"/> NEW
	<input checked="" type="checkbox"/> FINAL		<input type="checkbox"/> REVIEW

DESCRIPTIVE SUMMARY WITH CONCLUSIONS: (Include in this space references to data books, and to earlier related reports, patents and publications.)

Two methods have appeared in the literature recently for measuring the flux of organics from water to air (1,2). The predictive ability of these two methods was compared with some actual laboratory data. The analysis indicates that the method of Liss and Slater(2) is superior and can be used with a fair degree of confidence in making these kinds of estimations. The experimental data that is required is a knowledge of the vapor pressure and water solubility.



CRI NUMBER ↑

INTRODUCTION

There are many times when a knowledge of the flux of an organic chemical between air and water is valuable. For example, in estimating the movement of halocarbons in the biosphere it is necessary to know the rate at which the material moves between the atmosphere and the hydrosphere(3). In a different situation such as the spill of a chemical into a river, a knowledge of the rate of evaporation is fundamental in estimating the resulting concentration of the chemical as it moves downstream(4). Another example, discussed by Moyer(5) is the loss of organics from a tertiary treatment plant which is dependant on both degradation and evaporation mechanisms.

Two techniques for calculating this rate have recently appeared in the literature(1,2) and for convenience they will be identified in this report as A and B. It is the purpose of this report to compare these methods with some laboratory data.

METHOD A (MACKAY AND WOLKOFF) REF. 1

This method has been adequately discussed both in the original article and in a report by Moyer(5). The resulting equation for expressing the rate constant is shown in equation 1.

$$k = \left[\frac{E}{C_{is}} \frac{P_{is}}{P_w} \frac{M_i}{G} \frac{10^6}{P_w} \right] \text{hr}^{-1} \quad (1)$$

where G = grams of water containing the chemical
E = grams of water evaporating/hour
P_{is} = vapor pressure of pure material
P_w = vapor pressure of water
C_{is}^w = maximum solubility of organic (ppm)
M_i = molecular weight of organic
k = rate constant for evaporation

METHOD B (LISS AND SLATER) REF. 2

This method was originally developed to measure the flux of various gases across the air-sea interface. It essentially calculates the rate constant for the movement of a gas in either direction across this interface and is based on the assumption that the exchanging gas obey's Henry's law (this assumption is also true for Method A). Two equations (2 and 3) resulted from this derivation and are shown below.

$$K(\text{liquid}) = \frac{H k_g k_l}{H k_g + k_l} \quad (2)$$

$$K(\text{air}) = \frac{k_g k_l}{k_l + H k_g} \quad (3)$$

where K's are in units of (distance/time)
H is Henry's constant
(conc in gas phase)/(conc in liquid)
 k_g and k_l are exchange constants

The two exchange constants were estimated from field data taken in the ocean by Schooley(6). These had a mean value of 3000 cm hr⁻¹ for k_g (H₂O) and 20 cm hr⁻¹ for k_l (CO₂). In order to apply these constants to other materials, they should be multiplied by the ratio of the square roots of the molecular weights of H₂O and CO₂ with the gas in question.

The other parameter that needs to be evaluated is a number for Henry's constant. For slightly soluble materials the following relation holds in water.

$$p = \frac{X}{s} P_v \quad (4)$$

where p = partial pressure of the organic
P_v = vapor pressure of pure organic
X = weight fraction of organic in water
X_s = solubility of organic in water

$$\frac{\text{weight of chemical}}{\text{weight of air}} = \frac{P}{P_t} \times \frac{M}{M_a} \quad (5)$$

where P_t = partial pressure of air
 M^c = molecular weight of organic
 M_a = molecular weight of air ~29

Substituting the expression for p from (4) into (5) yields (6).

$$(\text{gms/cc}) \text{ air} = \frac{X}{X_s} \frac{P}{P_t} \frac{M}{29} \text{ density of air} \quad (6)$$

$$\text{or } H = \frac{(\text{gms/cc}) \text{ air}}{(\text{gms/cc}) \text{ water}} = \frac{P}{P_t} \frac{M}{29} \frac{\text{density of air}}{X_s} \quad (7)$$

For soluble materials: $p = X \frac{M_{H_2O}}{M} P_v$

Again, substituting this expression for p into (5) yields (8)

$$(\text{gms/cc}) \text{ air} = \frac{X}{M} \frac{18}{29} \frac{P_v}{P_t} \frac{M}{29} \quad (8)$$

which on rearranging gives (9).

$$H = \frac{(\text{gms/cc}) \text{ air}}{(\text{gms/cc}) \text{ water}} = \frac{18}{29} \frac{P_v}{P_t} \frac{\text{density of air}}{P_t} \quad (9)$$

Using these sets of equations Henry's constant was evaluated for several materials and compared with values reported in the literature. This comparison is shown in Table I and indicates that a reasonable estimate can be made with this procedure. To a first approximation these equations are obeyed provided the mole fraction of the solute is less than 0.02(8).

TEST DATA

The "Pollutional Evaluation of Compounds" edited by H. Alexander of Environmental Science(9) formed the basic data set by which these two methods could be evaluated. Essentially, the volatility measurements were made by gently aerating a liter

TABLE I.

COMPARISON OF CALCULATED VS
EXPERIMENTAL VALUE FOR HENRY'S CONSTANT

<u>Chemical</u>	<u>Henry's Constant</u>	
	<u>Exp.</u> ✓	<u>Calculated</u>
Methyl chloride	0.30	0.36
Methylene chloride	0.12	0.13
Chloroform	0.12	0.12
Carbon tetrachloride	0.91 1.08 ²	0.99
Ethylene dichloride	0.04	0.04
1,1,1-Trichloroethane	1.41	1.51
Vinyl chloride	50 ³	16 ⁴
Trichloroethylene	0.36	0.39
Perchloroethylene	0.82	0.87
Fluorotrichloromethane	33.3 ³ 5 ²	4.7

✓₁ All values except as indicated from Reference 7 were taken.

✓₂ Reference 2

✓₃ This value appears to be in error.

✓₄ The solubility data for vinyl chloride is questionable.

of solution containing 100 ppm of the organic and noting the change in chemical oxygen demand after four hours. The data on a number of compounds were collected in the report by Moyer(5). In order to compare the theoretical calculation with the experimental rate a selection of the data was made based on the following criteria:

1. Experimental data which had 0 or 100% removal in four hours was eliminated. This was done since determining a rate constant would not be very meaningful on this set.
2. Compounds whose solubility was less than 100 ppm were also deleted from the test set. This was necessary since the experiments of Alexander used 100 ppm as the initial concentration regardless of solubility.
3. Compounds where the vapor pressure or solubility were questionable were also eliminated from consideration.

This screening operation reduced the data set from 83 to 12. The chemicals along with the key chemical and physical properties are shown in Table II.

DETERMINATION OF RATE CONSTANTS AND
STATISTICAL EVALUATION OF THE RESULTS

Experimentally derived rate constant - The result in Alexander's report(9) is reported as % loss in four hours. For purposes of this calculation it was assumed that the rate of evaporation followed a simple first order reaction. With this assumption and knowing that the depth of the aeration cylinder was 15.5 inches a value for the rate constant in ft/hour was determined for each of the chemicals in Table II by using equation 10.

$$k = \frac{1}{4} \left(\ln \frac{C_0}{(C_0 - \text{loss in 4 hours})} \right) \frac{15.5}{12} \quad (10)$$

The results of this calculation are shown in Table III.

TABLE II

KEY CHEMICAL AND PHYSICAL PROPERTIES OF THE
DATA SET USED IN THIS STUDY

<u>NO.</u>	<u>Chemical</u>	<u>Mol. Wt.</u>	<u>Vap. Press.</u> <u>mm Hg</u>	<u>Solubility</u> <u>ppm</u>
1	1-Br,3-NO ₂ Benzene	170	0.07	10,000
2	3-Br,1-propanol	139	0.1	170,000
3	Methyl bromide	95	1400	13,000
4	Acetylene tetrabromide	344	0.3	650
5	Ethyl bromide	109	460	900
6	Ethylene dibromide	188	11.6	4,300
7	Epichlorohydrin	92.5	17.3	65,800
8	1,1,1-Trichloroethane	133.4	130.6	1,300
9	Triethylamine	101	7.0	73,000
10	4-t-butyl acetophenone	176	0.01	750
11	4-t-butyl phenol	150	0.046	1,000
12	Nitrobenzene	123	0.27	2,000

↓ These measurements were made at 25°C.

TABLE III

COMPARISON OF THEORETICALLY DERIVED RATE CONSTANTS WITH
THE EXPERIMENTAL VALUE OF THE CHEMICALS LISTED IN TABLE II

<u>Chemical</u> *	<u>Experimental</u>		<u>Theoretical</u>	
	<u>% loss</u>	<u>k(ft/hour)</u>	<u>A(ft/hr)</u>	<u>B(ft/hr)</u>
1	20	0.072	9.7×10^{-4}	.022
2	4	0.02	6.6×10^{-5}	1.6×10^{-4}
3	90	0.74	8.34	0.445
4	25	0.092	.129	0.110
5	86	0.63	45.4	0.442
6	80	0.519	0.413	0.236
7	21	0.076	0.019	0.053
8	70	0.38	10.93	0.38
9	15	0.052	0.0078	0.0219
10	75	0.45	0.0019	0.0042
11	12	0.04	0.005	0.013
12	36	0.14	0.0135	0.032

*Numbers refer to chemicals listed in Table II.

Theoretical Calculation

i) Method A - The experimental values for E and G in equation 1 are 0.27 gms/hour and 1000 gms respectively. Again, using 15.5" for the depth the expression in equation 11 can be used to evaluate the rate constant.

$$k = \left[\frac{0.27 \times 10^6 \times 15.5}{18 \times 1000 \times 12} \right] \left[\frac{P_{is} M_i}{C_{is} P_w} \right] \quad (11)$$

The results of this calculation are listed in Table III under Method A.

ii) Method B - Henry's constant is evaluated with equation 7 using a value of 0.001205 gms/cc for the density of air. By substituting this calculated value of H into equations 2 and 3 an estimation of the rate constant for both directions, namely air to water and water to air, may be made. For this calculation only the rate constant for water to air will be evaluated. This again is corrected for depth and the results are shown in Table III under Method B.

Statistics

The experimental rate constant (k_e) was treated as the dependant variable and regressed against the independent variable A or B. The results of these calculations are shown in the regression equations (12-14) along with the relevant statistics

$$k_e = 0.011 A + 0.178 \quad (12)$$

Standard error = 0.22
% variation explained 33.3

$$k_e = 1.21 B + 0.039 \quad (13)$$

Standard error = 0.15
% variation explained 69.5

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Equation 13 or Method B is by far the best description of the experimental data. Examination of the residual table (the amount by which the estimated k_e deviates from the experimental k_e) indicated one chemical that could be considered an outlier. This was 4-t-butyl acetophenone which had a much higher actual rate of evaporation than could be explained by equation 13. This would indicate one of two things: i) there is something wrong with either the reported solubility and vapor pressure or the experimentally reported loss. ii) there is something wrong with the model. Until we have more data there is no way of making a decision on which alternative is right. In the meantime this chemical was eliminated from the data set and the regression analysis repeated yielding equation 14. This is plotted in Figure 1.

$$\begin{aligned} k_e &= 1.37 B + 0.03 & (14) \\ \text{Standard error} &= 0.09 \\ \% \text{ variation explained} &= 88.7 \end{aligned}$$

Performing the regression on this data using A as the independent variable did not significantly improve the statistics from equation 12. The % variation explained went from 33% to 39%.

Before using equation 13 for predicting laboratory rate constants a measure of the variation to be expected in individual predictions must be determined. These ranges were calculated by means of the equations shown before and taken from Draper and Smith(10).

1. The standard error for the predicted mean value of k_e for a given B is given by equation 15.

$$\text{est s.e. } (\bar{Y}_k) = s \left\{ \frac{1}{n} + \frac{(X_k - \bar{X})^2}{\sum (X_i - \bar{X})^2} \right\}^{1/2} \quad (15)$$

where \hat{Y}_k is the predicted mean value for the rate constant evaluated at point k

- s = standard error of estimate for the regression
- n = number of data points used to establish the equation
- X_k = theoretical rate constant at point k
- \bar{X} = average value of X's

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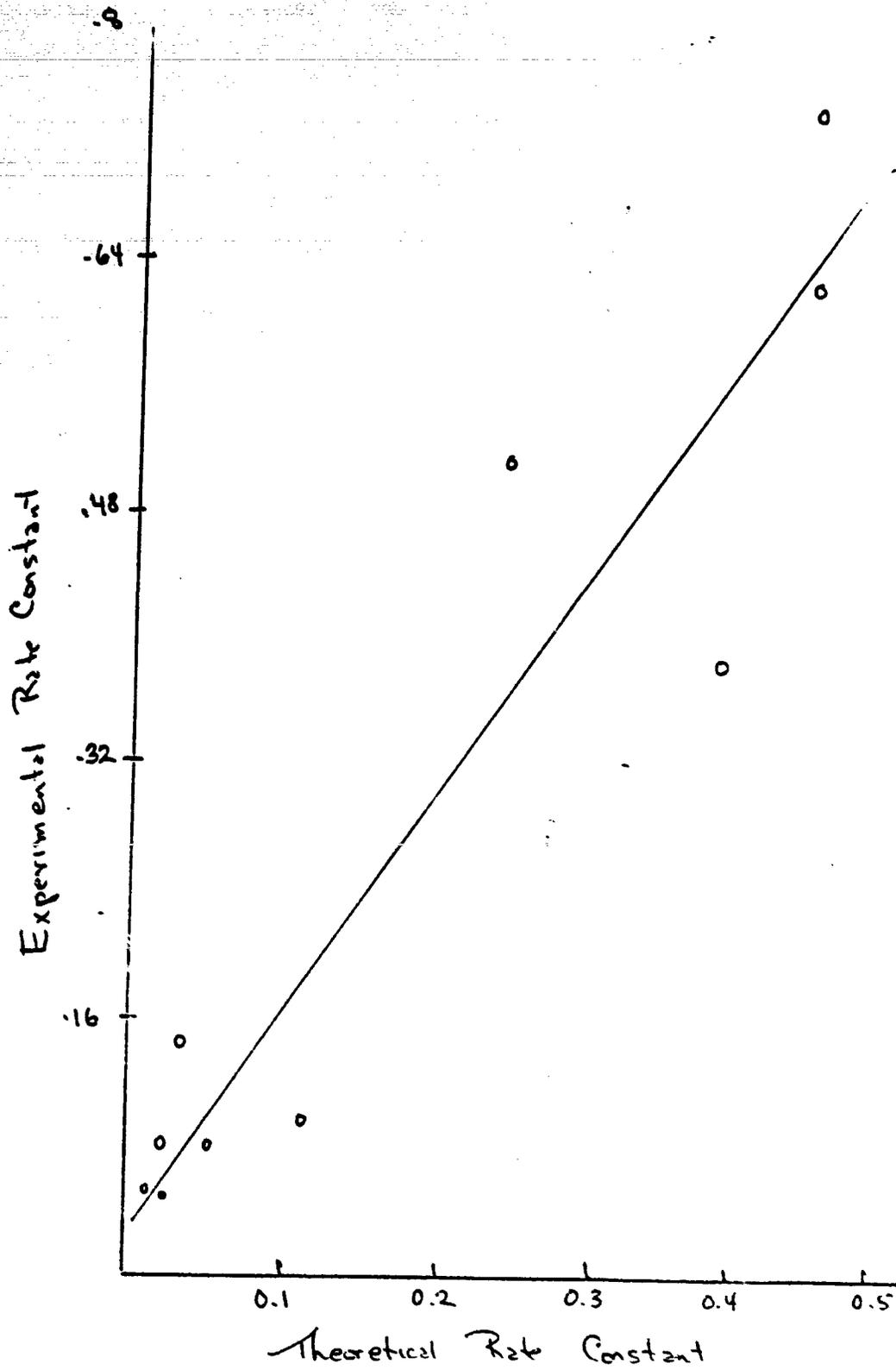


FIGURE 1

2. The standard error for a predicted value of an individual observation will have a broader range and is given by equation 16.

$$\hat{Y}_k \pm 2.68 \left[1 + \frac{1}{n} + \frac{(X_k - \bar{X})^2}{\sum (X_i - \bar{X})^2} \right]^{1/2} \quad (16)$$

where 2.68 is the 95% confidence value for the t statistic with 11 degrees of freedom.

These estimates were evaluated for the regression line and are shown in Figure 2.

In order to test the predictive capability of equation 14 it was necessary to go back to the data assembled by Moyer(5). This time the criteria used to make the selection were:

1. Solubility of 100 ppm or greater were still eliminated from further consideration.
2. A loss of 0 or 100% in four hours was included.

This last criteria necessitated placing a maximum and a minimum value on the theoretical rate constant. In other words if the calculated rate constant was equal to or greater than 0.55 than 100% loss in four hours could be expected. If the rate constant was equal to or less than 0.17, then 0% loss in four hours could be expected.

The selected chemicals along with the calculations are shown in Table IV. For the most part there is fairly good agreement between experimental and calculated result.

DISCUSSION

The method of Liss and Slater(2) does a good job of predicting rate of evaporation in laboratory experiments. The slope in equation 13 represents the difference in the laboratory conditions

FIGURE 2

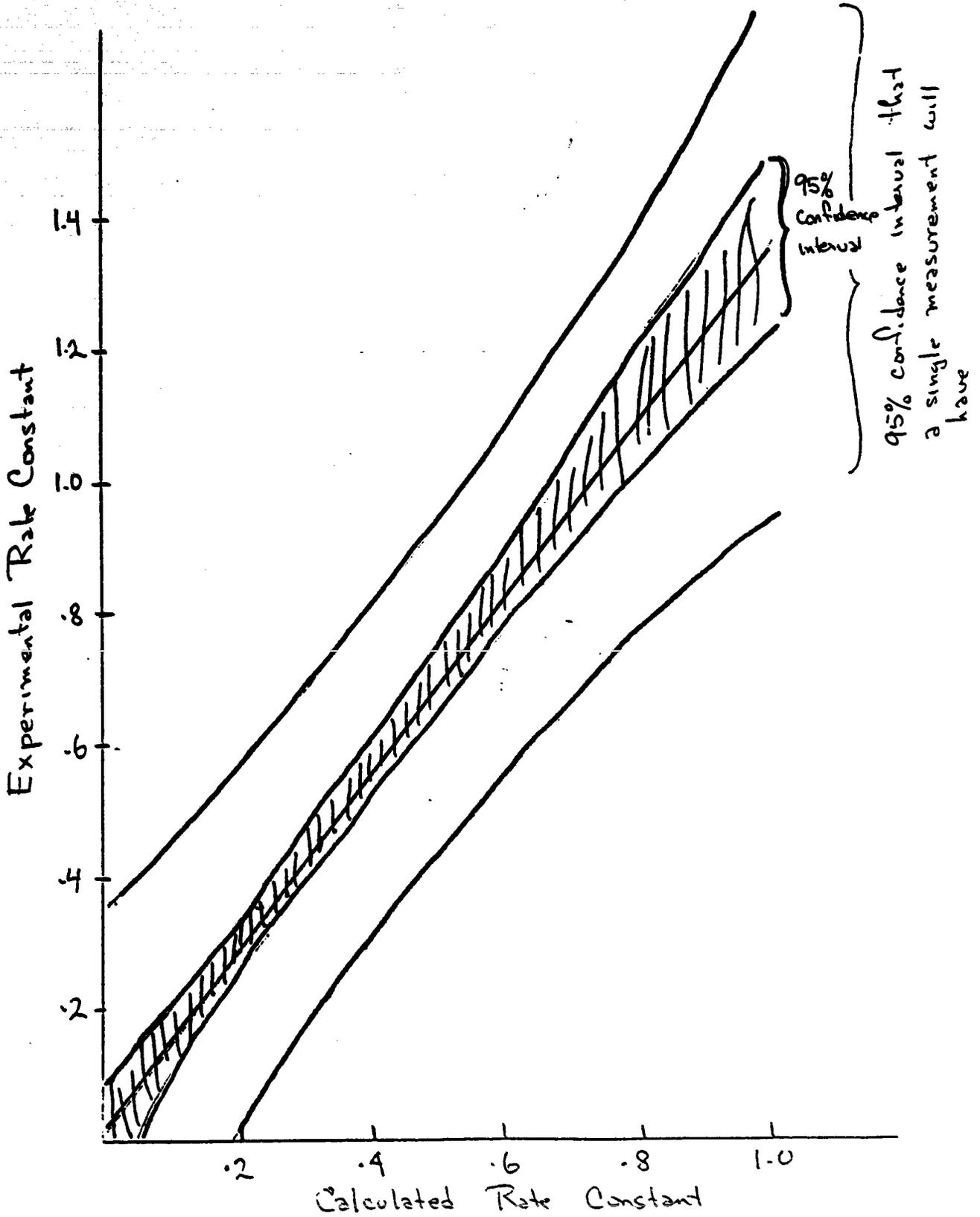


TABLE IV

SET OF CHEMICALS TO TEST PREDICTABILITY OF EQUATION 13

<u>Chemical</u>	<u>Mol. Wt.</u>	<u>Sol. ppm</u> <u>-measured at 25°C</u>	<u>V.P. mmHg</u> <u>at 25°C</u>	<u>% Loss</u> <u>Exp.</u>	<u>% Loss</u> <u>Est.</u>
1. Bromobenzene	159	446	4.1	100	94
2. Acrolein	56	215,000	56.1	0	0
3. Chloroform	119.5	7,100	26265	100	90
4. 1,2-Dichloroethane	99	865	105105	100	93
5. Trichloroethylene	131.4	300	800800	100	90
6. 4-t-butylcatechol	166	2,000	0.0028	0	0
7. 4-Chlorophenol	129	32,400	0.09	0	0
8. 2,4-Dichlorophenol	163	4,000	0.36	0	0
9. Benzene	78	1,790	95.2	100	100
10. α -Methylstyrene	118	560	3.13	100	89
11. Styrene	104	320	6312	100	90

as compared to the field data where Schooley(6) evaluated the exchange constants. If conditions in both places had been identical, the slope would be 1 with an intercept of 0.

A distinct advantage of the Liss and Slater(2) technique is that it generates rate constants for the flux of a chemical in both directions across the air water interface. If this estimation continues to be validated through experimental results, it will provide a convenient method for determining these types of rate constants.

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Heidi M. Hamel 5/6/83
SIGNATURE DATE