

# Haloethylene-Related Compounds of Industrial, Environmental, and Medical Significance

by Herbert S. Posner\* and Hans L. Falk\*

A broad-based literature survey was made for chemicals that contain either a haloethylene or a related substructure. Two hundred and sixty-two compounds, including synthetic intermediates, pesticides, solvents, drugs, food components, natural products, and metabolites, are grouped by their structures. Some are in current use or are bioavailable while little exposure is expected from others. As more biologic-response information is reported for small compounds of these types, it should become possible to select others for research on additional questions of structure-activity relationships.

Some of the compounds are widespread while others are not. Some are used or found in large amounts while others may be trace contaminants, minor or more major by-products of synthesis or isolation. The pesticides and solvents, for example, are knowingly and often deliberately released to the environment, sometimes in very large quantities. Inadvertent release also occurs, sometimes referred to as fugitive emission. Food contaminants and drugs are directly accessible to humans. Sparsely distributed natural products could be accessible to humans, for example, via the food chain. Some of the compounds in food may be formed during preparation, storage or metabolically. Last, the haloethylene function has often been synthesized into compounds in order to achieve desired biologic activities.

There are many types and degrees of relatedness of structure, depending upon atomic dimensions and stereochemical, polar, resonance, and other factors. Furthermore, for some chemical series, biologic responses are continuously variable while, in other cases, it is not uncommon that qualitatively different types of response occur with apparently very close homologs. Genetic, metabolic, and behavioral factors affecting response must also be considered. Thus, safety or hazard cannot yet be predicted conclusively by apparent relatedness of structure alone. Also, since the tables are noncomprehensive, some relevant compounds have likely been omitted. The haloalkanes, for example, are not here because of their large number, despite the knowledge that some are either metabolized or nonbiologically converted to haloalkenes.

## Introduction

Vinyl chloride and some lower homologs have drawn attention in the past few years because of demonstrated or potential health hazards. A sufficient number of these have come into question so that a broad survey for this functional group in larger molecules was undertaken in order to permit an extended consideration of structure-activity relationships.

There are many subtleties of closeness of structure. Also, initially related or unrelated compounds

may become, respectively, unrelated or related by either metabolic or nonbiologic reactions. While Tables 1-6 are broad in scope, they are not comprehensive. There are at least three types of omissions: inadvertent; purposeful, because of the large number of compounds within a series (for example, the many alkanes that may be converted to alkenes); and those omitted because of an inability to be comprehensive without diluting the list with compounds for which there is scant reported use or human exposure.

The physicochemical factors of both the chemicals and exposed biologic species can be of immense importance in the control of biologic uptake, distribution, metabolism, storage, and subsequent excretion, secretion, or exhalation of the com-

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Table 1. Haloalkenes

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
Ethenes					
$\text{CH}_2=\text{CHX}$	X				
	-Cl	1-1	ethene, chloro- (vinyl chloride, vinyl chloride monomer, chloroethylene, VC, VCM)	Polymer and other synthesis; propellant; refrigerant	(1,2,9)
	-Br	1-2	ethene, bromo- (vinyl bromide)	Polymer and other synthesis; flame retardant	(1)
	-F	1-3	ethene, fluoro- (vinyl fluoride)	Polymer and other synthesis	(1)
	-I	1-4	ethene, iodo- (vinyl iodide)	(Not found)	(10)
	-Cl	1-5	ethene, 1,1-dichloro- (vinylidene chloride, 1,1-dichloroethylene, <u>asym</u> -dichloroethylene)	Polymer and other synthesis	(1,2,9)
	-Br, -F or -I	1-6 to 1-8	(Named as in 1-5)	(Br and F) Polymer and other synthesis; (I) not found	(1,10,11)
	-Cl	1-9	ethene, 1,2-dichloro-, (trans-) (sym-trans-dichloroethylene, <u>trans</u> -acetylene dichloride)	Synthesis; solvent (trans- and <u>cis</u> , <u>trans</u> - mixture used more than <u>cis</u> -); retarding fermentation	(1,2,12)
	-Br, -F or -I	1-10 to 1-12	(Named as in 1-9)	(Not found)	(2,10,11)
	-Cl	1-13	ethene, 1,2-dichloro-, ( <u>cis</u> -) (named as in 1-9, but <u>cis</u> -)	Synthesis	(1)
	-Br, -F or -I	1-14 to 1-16	(As in 1-9, but <u>cis</u> -)	(Not found)	(10,11)
	-Cl	1-17	ethene, trichloro- (1,1,2-trichloroethylene, acetylene trichloride, ethylene trichloride, ethinyl trichloride, tri, TCE)	Synthesis; solvent; registered pesticide (fumigant); drug (anesthetic);	(1,2,3,7)

(continued)

Table 1 (cont.)

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
X					
$\text{CH}_2=\text{CX}_2$	-Br, -F or -I	1-18 (Named as in 1-17) to 1-20		solvent dyeing; cleaning and drying metal; flushing liquid oxygen (Not found)	(10,11)
$\text{CX}_2=\text{CX}_2$	-Cl	1-21	ethene, tetrachloro- (perchloroethylene, ethylene tetrachloride, perc)	Polymer and other synthesis; solvent (vapor degreasing, dry cleaning); registered pesticide (vermifuge); heat exchange fluid	(1,2,9)
	-Br, -F or -I	1-22 to 1-24	[As 1-21 and also: (F) TFE, (I) ethylene periodide, diiodoform, iodoethylene]	(Br and F) Polymer and other synthesis; (I) drug (surgical dusting powder, antiseptic ointment); pesticide (fungicide)	(1,2,3)
$\text{CH}_2=\text{CBrCl}$	--	1-25	ethene, 1-bromo-1-chloro-	Fire retardant	(13)
$\text{CHCl}=\text{CF}_2$	--	1-26	ethene, 1-chloro-2,2-difluoro-	Polymer synthesis; metabolite of halothane ( $\text{CHBrCl}-\text{CF}_3$ )	(14)
$\text{CClF}=\text{CF}_2$	--	1-27	ethene, chlorotrifluoro- (monochlorotrifluoroethylene, trifluorovinyl chloride, CFE, CTFE)	Polymer synthesis	(1)
$\text{CBrF}=\text{CF}_2$	--	1-28	ethene, bromotrifluoro- (BFE)	Polymer synthesis	(1)
$\text{CBrCl}=\text{CF}_2$	--	1-29	ethene, 1-bromo-1-chloro-2,2-difluoro-	Metabolite of halothane ( $\text{CHBrCl}-\text{CF}_3$ )	(14)
$\text{CCl}_2=\text{CF}_2$	--	1-30	ethene, 1,1-dichloro-2,2-difluoro-	Polymer and other synthesis	(15)
$\text{CBrI}=\text{CBrI}$	--	1-31	ethene, 1,2-dibromo-1,2-diiodo- (sym-dibromodiiodoethylene)	Synthesis	(1)

(continued)

Table 1 (cont.)


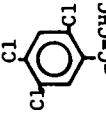
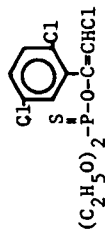
Structure	Substituents		Compound No.	Names	Present or past uses; sources	References
Propenes						
$RCR_1=CHCl$	R	$R_1$	X			
	$CH_3-$	--	--	1-32 1-propene, 1-chloro- (propenyl chloride)	(Not found)	(5)
	$CH_2OH-$	--	--	1-33 1-propene-3-ol, 1-chloro- ( <del>4</del> chloro-allyl alcohol, 1-chloro-3-hydroxypropene, 3-chloro-2-propene-1-ol)	Hydrolytic product of 1,3-dichloropropene (compound No. 1-34) in wet soil	(16)
$RCR_1=CHCl$	$CH_2Cl-$	--	--	1-34 1-propene, 1,3-dichloro- (1,3-dichloropropylene, 3-chloropropenyl chloride, 1,3-D)	Synthesis; registered pesticide (in mixture with 1,2-dichloropropene, dichloropropenes and/or chloropicrin -- soil fumigant and nematocide)	(1,2,3,17)
	$CH_2Br-$	--	--	1-35 1-propene, 3-bromo-1-chloro- (CBP-55)	Pesticide (soil fumigant)	(3)
$RCCl=CH_2$	$CH_3-$	--	--	1-36 propene, 2-chloro- (isopropenyl chloride)	Polymer and other synthesis	(1,5)
	$CH_2Cl-$	--	--	1-37 1-propene, 2,3-dichloro-	Contaminant of DD (see compound No. 1-34)	(18)
$CX_3-CX=CX_2$	--	--	-Cl	1-38 propene, 1,1,2,3,3,3-hexachloro- (perchloropropylene)	Solvent; plasticizer; hydraulic fluid	(1)
Butenes						
	--	--	-F	1-39 propene, 1,1,2,3,3,3-hexafluoro- (perfluoropropylene, HFP)	Polymer synthesis	(1)
$RCR_1=CHX$	$CH_3-$	$-CH_3$	-Cl	1-40 1-propene, 1-chloro-2-methyl- ( <del>4</del> chloroisobutylene, $\beta,\beta$ -dimethylvinyl chloride, isocrotyl chloride)	Synthesis	(2)

(continued)

Table 1 (cont.)

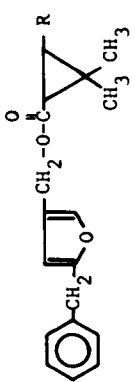
Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
$R_1R_2=CHX$	R $R_1$ X CH <sub>2</sub> Cl-CHCl-	1-41	1-butene, 1,3,4-trichloro-	Contaminant of vinyl chloride via oxychlorination synthesis	(19)
$RCX=CH_2$	---	1-42	1-butene, 2,3,4-trichloro-	Contaminant of vinyl chloride via oxychlorination synthesis	(19)
$CH_3-CCl=CH-CH_2Cl$	CH <sub>2</sub> =CH <sub>2</sub> -	1-43	1,3-butadiene, 2-chloro- (chloroprene, 2-chlorobutadiene)	Synthesis of polychloroprene (neoprene)	(1)
$CH_2=CCl-CH=CH_2$	---	1-44	2-butene, 1,3-dichloro-	Contaminant of chloroprene via acetylene synthesis	(1,20)
$CH_2Cl-CH=CCl-CH_2Cl$	---	1-45	2-butene, 1,2,4-trichloro-	Contaminant of vinyl chloride via oxychlorination synthesis	(19)
$CF_3-C=CF_2$	---	1-46	1-propene, 1,1,3,3,3-pentafluoro-2-trifluoromethyl- (octafluoroisobutene, perfluoroisobutene, PFIB)	Most toxic fluoroalkene tested to date	(21)
$CCl_2=CCl-CCl=CCl_2$	---	1-47	1,3-butadiene, 1,1,2,3,4-hexachloro- (hexachlorobutadiene, perchlorobutadiene, HCB, C-46)	Solvent; heat transfer liquid; transformer and hydraulic fluid; by-product of hexachlorobenzene synthesis	(1,22)
$RCX=CR_1X$	CH <sub>2</sub> OH- -CH <sub>2</sub> OH	1-48	2-butene-1,4-diol, 2,3-dibromo- (dibromobutenediol)	Flame retardant	(13)
	CF <sub>3</sub> -	1-49	2-butene, 2,3-dichloro-1,1,4,4,4-hexafluoro- (DCHFB, HFCB)	A toxic impurity of halothane (CHBrCl-CF <sub>3</sub> )	(21)
	CF <sub>3</sub> -	1-50	2-butene, 1,1,1,2,3,4,4,4-octafluoro- (perfluoro-2-butene)	Polymer and other synthesis	(1)

(continued)

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
Organophosphate and sulfonyl compounds					
$(R)_2-P-OR_1$	R	R <sub>1</sub>			
	C <sub>2</sub> H <sub>5</sub> O-	-CH=CHCl	1-51	phosphoric acid, 2-chloroethenyl diethyl ester [2-chlorovinyl diethyl phosphate, OS-1836; compounds No. 1-51 to 1-57 have also been named with the vinyl designation or as phosphate (or phosphorothioate) derivatives]	Pesticide (insecticide) (3)
	C <sub>2</sub> H <sub>5</sub> O-		1-52	phosphoric acid, 2-chloro-1-(2,4-dichlorophenyl)ethenyl diethyl ester (chlorfenvinfos, chlofenvinfos, as in 1-51)	Registered pesticide (insecticide) (2,3)
	CH <sub>3</sub> O-		1-53	phosphoric acid, 2-chloro-1-(2,4,5-trichlorophenyl)ethenyl dimethyl ester (stirofos, tetrachlorvinfos, CVMP, (as in 1-51))	Registered pesticide (insecticide) (2,3)
	C <sub>2</sub> H <sub>5</sub> O-	-CH <sub>2</sub> -CHCl-O-CH=CCl <sub>2</sub>	1-54	phosphoric acid, 1-(2-chloroethoxy)-2,2-dichloroethenyl diethyl ester (phosphinon, as in 1-51)	Pesticide (insecticide) (3)
	CH <sub>3</sub> O-	-CH=CCl <sub>2</sub>	1-55	phosphoric acid, 2,2-dichloroethenyl dimethyl ester (dichlorvos, chlorvinfos, DDVP, as in 1-51)	Veterinary drug (anthelmintic, insecticide); registered pesticide (insecticide, fumigant) (1,2,3)
$CH_2Cl-CH_2-O-P(=O)(OC_2H_5)_2$	--	--	1-56	phosphoric acid, 2-chloroethyl 2,2-dichloroethenyl ethyl ester (as in 1-51)	Pesticide (insecticide) (3)
	--	--	1-57	phosphorothioic acid, O-[2-chloro-1-(2,5-dichlorophenyl)ethenyl] O,O-diethyl ester (as in 1-51)	Pesticide (insecticide) (3)
$R-S(=O)_2-CCl=CHCl$	CH <sub>3</sub> -	--	1-58	ethene, 1,2-dichloro-1-methylsulfonyl-[1,2-dichloro-1-(methylsulfonyl)ethylene, D-113]	Pesticide (fungicide) (5)

(continued)

Table 1 (cont.)

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
$R-\overset{\text{O}}{\parallel}{S}-\text{CCl}=\text{CHCl}$	$R$ $C_4H_9-$	1-59	butane, 1-((1,2-dichloroethenyl)sulfonyl)-(1,2-dichloro-1-butylsulfonyl)ethylene, D-121)	Pesticide (fungicide)	(3)
Thiocarbamates					
$(R)_2N-\overset{\text{S}}{\parallel}{C}-S-\text{CH}_2R_1$	$R_1$ $C_2H_5-$	1-60	carbamodithioic acid, diethyl-, 2-chloro-2-propenyl ester (sulfalate, thioallate, 2-chloroallyl N,N-diethyl-dithiocarbamate, CDEC)	Registered pesticide (herbicide)	(1,3)
$(R)_2N-\overset{\text{O}}{\parallel}{C}-S-\text{CH}_2R_1$	$R_1$ $(CH_3)_2CH-$	1-61	carbamothioic acid, bis(1-methylethyl)-S-(2,3-dichloro-2-propenyl) ester [diallate, S-(2,3-dichloroallyl)diisopropylthiocarbamate, DATC, 2,3-DCDT]	Registered pesticide (herbicide)	(1,2,3)
Pyrethroids					
	$(CH_3)_2CH-$	1-62	carbamothioic acid, bis(1-methylethyl)-S-(2,3,3-trichloro-2-propenyl) ester [triallate, S-(2,3,3-trichloroallyl)diisopropylthiocarbamate]	Registered pesticide (herbicide)	(1,3)
R					
$-CH=CHCl$	$R$	1-63	cyclopropanecarboxylic acid, 3-(2-chloroethenyl)-2,2-dimethyl-, (5-phenylmethyl)-3-furanyl)methyl ester	Pesticide (insecticide)	(23,24)
$-CH=CCl_2$	$R$	1-64	cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, (5-phenylmethyl)-3-furanyl)methyl ester	Pesticide (insecticide)	(23-25)
$-CH=CBr_2$	$R$	1-65	cyclopropanecarboxylic acid, 3-(2,2-dibromoethenyl)-2,2-dimethyl-, (5-phenylmethyl)-3-furanyl)methyl ester (bromethrin)	Pesticide (insecticide)	(23-26)
$-CH=CF_2$	$R$	1-66	cyclopropanecarboxylic acid, 3-(2,2-difluoroethenyl)-2,2-dimethyl-, (5-phenylmethyl)-3-furanyl)methyl ester (fluorethrin)	Pesticide (insecticide)	(25,27)

(continued)

Table 1 (cont.)

Structure	Substituents	Compound No.	Names	Present or past uses, sources	References
	R <sub>1</sub> R				
	-CH <sub>2</sub> -	1-67	cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, 3-(phenoxyphenyl)methyl ester (permethrin, NRDC 143, dl-cis,trans; biopermethrin, NRDC 147, d-trans-)	Pesticide (insecticide)	(24,25, 28,29)
	CN -CH-	1-68	cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester (NRDC 149, IRS, 3RS, 4RS)	Pesticide (insecticide)	(24,25)
	CN -CH-	1-69	cyclopropanecarboxylic acid, 3-(2,2-dibromoethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester [decamethrin, NRDC 161, [S]-cyano-3-phenoxybenzyl cis-(1R,3R) 2,2-dimethyl-3-(2,2-dibromovinyl)cyclopropane carboxylate -- most active compound and isomer to date]	Pesticide (insecticide)	(24,25, 30-32)
Barbiturates	R				
	-CH <sub>2</sub> -CH=CH <sub>2</sub>	1-70	2,4,6(1H,3H,5H)-pyrimidinetrione, 5-(2-bromo-2-propenyl)-5-(2-propenyl)-[brallobarbital, 5-allyl-5-(2-bromoallyl)barbituric acid]	Drug (hypnotic)	(2)
	CH <sub>3</sub> -CH-CH <sub>2</sub> -CH <sub>3</sub>	1-71	2,4,6(1H,3H,5H)-pyrimidinetrione, 5-(2-bromo-2-propenyl)-5-(1-methylpropyl)-[butallylonal, sonbutal, 5-(2-bromoallyl)-5-sec-butylbarbituric acid]	Drug (hypnotic)	(2,33)
	CH <sub>3</sub> -CH-CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>3</sub>	1-72	2,4,6(1H,3H,5H)-pyrimidinetrione, 5-(2-bromo-2-propenyl)-5-(1-methylbutyl)-[5-(2-bromoallyl)-5-(1-methylbutyl)barbituric acid, R-239]	Drug (hypnotic, sedative)	(2)
	-CH(CH <sub>3</sub> ) <sub>2</sub>	1-73	2,4,6(1H,3H,5H)-pyrimidinetrione, 5-(2-bromo-2-propenyl)-5-(1-methylethyl)-[propallylonal, 5-(2-bromoethyl)-5-isopropylbarbituric acid]	Drug (hypnotic, sedative)	(2)

(continued)



Table 1 (cont.)

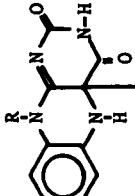
Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
Amino acids and fatty acids					
$\text{R}$ $\text{NH}_2$ $\text{HOOC}-\text{CH}-\text{CH}_2-\text{SR}$	$-\text{CCl}=\text{CHCl}$	1-74	L-cysteine, S-(1,2-dichloroethenyl)-[S-(1,2-dichlorovinyl)-L-cysteine, DCVC]	In vitro reaction product of trichloroethene with cysteine	(34-36)
	$-\text{CCl}=\text{CCl}-\text{S}-\text{CH}_2-\overset{\text{NH}_2}{\text{C}}-\text{COOH}$	1-75		In vitro reaction product of tetrachloroethene with cysteine	(34,35)
	$-\text{CCl}=\text{CCl}_2$	1-76	L-cysteine, S-(1,2,2-trichloroethenyl)-	In vitro reaction product of tetrachloroethene with cysteine	(34,35)
$\text{CH}_3-(\text{CH}_2)_7-\text{Cl}-\text{Cl}-(\text{CH}_2)_7-\text{COOC}_2\text{H}_5$		1-77	13-docosenoic acid, 13,14-difido-, ethyl ester (iodobrassid, ethyl diiodobrassidate)	Drug (iodine source)	(2)
Others and isosteres					
$\text{Cl}_2\text{AsCH}=\text{CHCl}$	--	1-78	arsenous dichloride, (2-chloroethenyl)-[Lewisite, dichloro(2-chlorovinyl)arsine, chlorovinyl arsine dichloride]	Poison gas	(1,2)
$\text{CH}_3-\overset{\text{C}\equiv\text{CH}}{\text{C}}-\text{CH}=\text{CHCl}$	--	1-79	1-penten-4-yn-3-ol, 1-chloro-3-ethyl-(ethchlorvynol, ethyl $\beta$ -chlorovinyl ethynyl carbinol	Drug (hypnotic, sedative)	(1,2,7,8)
$\left[ \begin{array}{c} \text{CH}_2-\text{CH}=\text{CHCl} \\ \text{N} \\ \text{N} \end{array} \right] \text{Cl}^-$	--	1-80	3,5,7-triaza-1-azoniatricyclo(3.3.1.1.1-(3,7))decane, 1-(3-chloro-2-propenyl)-, chloride [1-(3-chloroallyl)-3,5,7-triaza-1-azoniaadamantane chloride, N-(3-chloroallyl)hexamminium chloride]	Bactericide (used in latexes, paint, floor polish, joint cement, adhesives, inks, star-ches, etc.)	(1,2)
$(\text{CH}_3)_2\text{S}-\text{CH}_2-\overset{\text{O}}{\parallel}{\text{C}}-\text{NH}-\text{C}-\text{CH}_2-\text{S}-\text{CH}=\text{CCl}-\text{CH}_3$	--	1-81	4-thia-1-azabicyclo(3.2.0)heptane-2-carboxylic acid, 6(((3-chloro-2-butenyl)thio)acetyl)amino)-3,3-dimethyl-7-oxo, monopotassium salt, (2S-(2R,5R-6R)) (penicillin S potassium)	Drug (antibiotic)	(2)
	--	1-82		Experimental irreversible inhibitor of flavin-linked monamine oxidases	(37)
$\text{NH}-\text{CH}_2-\text{CH}=\text{CHBr}$					(continued)

Table 1 (cont.)

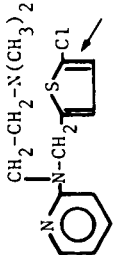
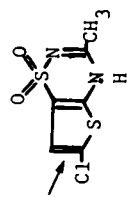


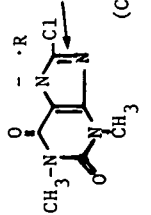
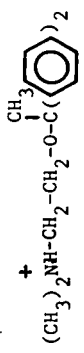
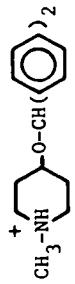
Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
	R	1-83	benzenecarbohydrazonyl chloride, N-(2,4,6-trichlorophenyl)- [benzoyl chloride (2,4,6-trichlorophenyl)hydrazone]	Pesticide (acaricide)	(18)
	H-	1-84	benzenecarbohydrazonyl chloride, 4-methyl-N-phenyl- (p-toluy) chloride phenylhydrazone)	Experimental drug	(38)

Table 2. Halocycloalkenes and ring-conjugated haloalkenes

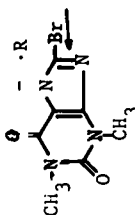
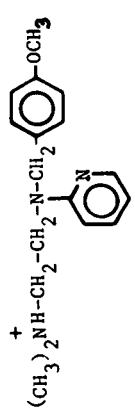
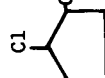
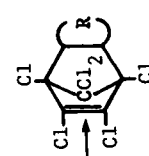
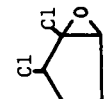
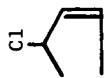


Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
	R	2-1	1,3-cyclopentadiene, 1,2,3,4,5,5-hexachloro- (perchlorocyclopentadiene, C-56)	Synthesis of resins, dyes, pesticides, drugs; registered pesticide (fumigant)	(1,3)
	-Cl	2-2	bis-2,4-cyclopentadien-1-yl, 1,1',2,2',3,3',4,4',5,5'-decachloro- [dienochlor, bis(pentachlorocyclopentadienyl)]	Registered pesticide (acaricide)	(1,3)
	--	2-3	1H-pyrrole, 3-chloro-4-(3-chloro-2-nitrophenyl)- (pyrrolnitrin)	Drug (antifungal)	(2)
	--	2-4	1H-pyrrole, 2,3,4,5-tetraiodo- (iodopyrrole)	Drug (topical antiseptic; veterinary -- topical antiseptic in female reproductive tract)	(2)
	-H	2-5	ergoline-8-carboxamide, 2-bromo-9,10-dihydro-N,N-diethyl-6-methyl, (8 $\beta$ -bromo-LSD, D-2-bromolysergic acid diethylamide, bromolysergide)	Experimental serotonin antagonist	(2,39)
	-CH <sub>3</sub>	2-6	ergoline-8-carboxamide, 2-bromo-9,10-dihydro-N,N-diethyl-1,6-dimethyl- (8 $\beta$ )	Experimental psychotropic drug	(39)

(continued)

Table 2 (cont.)

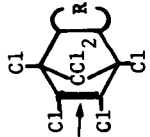

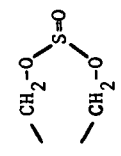
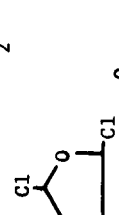
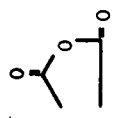
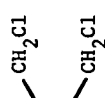
Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
	--	2-7	1,2-ethanediamine, N-(5-chloro-2-thienylmethyl)-N',N'-dimethyl-N-2-pyridinyl- (chlorothen, chloropyri- lene, chloromethapyri- line)	Drug (antihistaminic)	(2)
	--	2-8		Experimental antihyper- tensive agent	(40)
	--	2-9	thiophene, tetrachloro- (perchloro- thiophene, TCTP, TD-183)	Registered pesticide (soil fumigant, insecticide, nematocide)	(1,3)
	--	2-10	5-isoxazoleacetic acid, $\alpha$ -amino-3-chloro-4,5-dihydro-	Experimental antineo- plastic drug; <u>Strepto- myces sviveus</u> (fungi)	(41)
	--	2-11	1H-purine-2,6-dione, 8-chloro-3,7-dihydro-1,3-dimethyl-, compound with 2-(diphenylethoxy)-N,N-dimethyleth- anamine (1:1) (dimenhydrinate, com- pounds 2-11 to 2-13 have also been named as the 8-chlorotheophylline com- pound with the positively charged molecule)	Drug (human and veteri- nary antiemetic)	(2,7,8)
	--	2-12	1H-purine-2,6-dione, 8-chloro-3,7-dihydro-1,3-dimethyl-, compound with 2-(1,1-diphenylethoxy)-N,N-dimethyleth- anamine (1:1) (mephenhydrinate, also named as in 2-11)	Drug (tranquilizer)	(39)
	--	2-13	1H-purine-2,6-dione, 8-chloro-3,7-dihydro-1,3-dimethyl-, compound with 4-(diphenylethoxy)-1-methylpiperidine (1:1) (piprinhydrinate, also named as in 2-11)	Drug (antihistaminic, antiemetic)	(2)

(continued)

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
	R + NH <sub>3</sub> -C(CH <sub>3</sub> ) <sub>2</sub> -CH <sub>2</sub> OH	2-14	1H-purine-2,6-dione, 8-bromo-3,7-dihydro-1,3-dimethyl-, compound with 2-amino-2-methyl-1-propanol (pamabrom; compounds No. 2-14 and 2-15 have also been named as the 8-bromotheophyllinate compound with the positively charged molecule)	Drug (diuretic)	(2,8)
	(CH <sub>3</sub> ) <sub>2</sub> NH-CH <sub>2</sub> -CH <sub>2</sub> -N-CH <sub>2</sub> -N-CH <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> -OCH <sub>3</sub>	2-15	1H-purine-2,6-dione, 8-bromo-3,7-dihydro-1,3-dimethyl-, compound with N-((4-methoxyphenyl)methyl)-N',N'-dimethyl-N-2-pyridinyl-1,2-ethanediamine (1:1) (pyrabrom, also named as in 2-14)	Drug (antihistaminic)	(2,7)
		2-16	4,7-methano-1H-indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro- (chlordane, octachlor)	Veterinary drug and registered pesticide (insecticide, acaricide)	(1,2,3)
		2-17	2,5-methano-2H-indeno(1,2-b)oxirene, 1a,2,3,4,5,6a,7,7-octachloro-1a,1b,5,5a,6,6a-hexahydro- (oxychlordane, chlordane epoxide)	Metabolite of chlordane (compound No. 2-16)	(42)
		2-18	4,7-methano-1H-indene, 1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro- (heptachlor, 3-chlorochlordane)	Registered pesticide (insecticide)	(1,2,3)
		2-19	2,5-methano-2H-indeno(1,2-b)oxirene, 2,3,4,5,6,7,7-heptachloro-1a,1b,5,5a,6,6a-hexahydro- (heptachlor epoxide)	Metabolite of heptachlor (compound No. 2-18); insecticide activity	(1,3)
		2-20	4,7-methano-1H-indene, 4,5,6,7,8,8-hexachloro-3a,4,7,7a-tetrahydro- (chlordane)	Synthesis of chlordane	(3)
		2-21	1,4:5,8-dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro- (1 $\alpha$ ,4 $\alpha$ ,4 $\beta$ ,5 $\alpha$ ,8 $\alpha$ ,8 $\beta$ )- (aldrin, HHDN)	Registered pesticide (insecticide)	(1,2,3)

(continued)

Table 2 (cont.)

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
	R				
(as in 2-21)		2-22	1,4:5,8-dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro- (1 $\alpha$ ,4 $\alpha$ ,4 $\beta$ ,5 $\beta$ ,8 $\beta$ ,8a $\beta$ )- (isodrin, the 5 $\beta$ ,8 $\beta$ isomer of compound No. 2-21)	Pesticide (insecticide)	(1,2,3)
		2-23	2,7:3,6-dimethanonaphth(2,3-b)oxirene, 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-, (1 $\alpha\alpha$ ,2 $\beta$ ,2 $\alpha\alpha$ ,3 $\beta$ ,6 $\alpha$ ,6 $\alpha$ ,7 $\beta$ ,7 $\alpha\alpha$ )- (dieldrin, aldrin epoxide, HEOD)	Veterinary drug and registered pesticide (insecticide)	(1,2,3)
(as in 2-23)		2-24	2,7:3,6-dimethanonaphth(2,3-b)oxirene, 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-, (1 $\alpha\alpha$ ,2 $\beta$ ,2 $\alpha\alpha$ ,3 $\beta$ ,6 $\alpha$ ,6 $\alpha$ ,7 $\beta$ ,7 $\alpha\alpha$ )- (endrin, the 2 $\alpha\alpha$ ,3 $\alpha$ ,6 $\alpha$ ,6 $\alpha$ isomer of compound No. 2-23)	Registered pesticide (insecticide)	(1,2,3)
		2-25	6,9-methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide (endosulfan, chlorthiepin)	Registered pesticide (insecticide)	(1,2,3)
		2-26	4,7-methanoisobenzofuran, 1,3,4,5,6,7,8,8-octachloro-1,3,3a,4,7,7a-hexahydro- (isobenzan)	Registered pesticide (insecticide)	(1,2,3)
		2-27	4,7-methanoisobenzofuran-1,3-dione, 4,5,6,7,8,8-hexachloro-3a,4,7,7a-tetrahydro- (chlorendic anhydride, HET anhydride)	Flame retardant for polyester resins and other synthesis; hardening epoxy resins; source of chlorendic acid	(1,2)
		2-28	bicyclo(2.2.1)hept-2-ene, 1,2,3,4,7,7-hexachloro-5,6-bis(chloromethyl)- (chlorbicyclin)	Pesticide (insecticide, acaricide)	(3)

(continued)

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
Di- and triphenylethylenes					
	R Cl	X -Cl	benzene, 1,1'-(dichloroethylenylidene)-bis(4-chloro)- [DDE, 1,1-dichloro-2,2-di(p-chlorophenyl)ethylene]	Contaminant and metabolite of DDT	(1,3)
	(C <sub>2</sub> H <sub>5</sub> )N-CH <sub>2</sub> -O- CH <sub>3</sub> O- -H	-Cl -OCH <sub>3</sub> -H	ethanamine, 2-(4-(2-chloro-1,2-diphenylethylenyl)phenoxy)-N,N-diethyl- (clomiphene, chloramiphen)	Drug [gonad stimulation (ovulation induction)]	(2,7,8,33)
	CH <sub>3</sub> O- -O-C-CH <sub>3</sub>	-OCH <sub>3</sub> -OCH <sub>3</sub>	benzene, 1,1',1''-(1-chloro-1-ethenyl-2-ylidene)tris(4-methoxy)- [chlorotri-anisole, chlorotris(p-methoxyphenyl)ethylene]	Drug (estrogen)	(2,7,8,33)
	CH <sub>3</sub> -C(=O)- -O-C-CH <sub>3</sub>	-O-C-CH <sub>3</sub>	phenol, 4,4'-( $\alpha$ -bromobenzylidene)methylene)di-, diacetate (8CI) 4,4'-( $\beta$ -bromostyrylidene)diphenol diacetate)	Drug (estrogen)	(2)
	C <sub>2</sub> H <sub>5</sub> - -H	-H	benzene, 1-(2-bromo-1,2-diphenylethenyl)-4-ethyl- (broparestrol) B.D.P.E.)	Drug (estrogen, used in dermatology)	(2)

Table 3. Haloalkene and halocycloalkene compounds from Rhodophyta species (red algae) and from a species that feeds on these (*Aplysia californica*; mollusc)

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
Monoterpenes					
	--	3-1	<i>Plocamium cartilagineum</i> ; <i>Aplysia californica</i>		(43,44)
	--	3-2	<i>Plocamium</i> sp.; <i>A. californica</i>		(43,44)

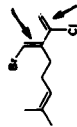
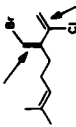
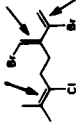
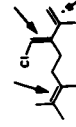
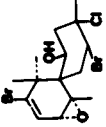
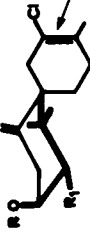
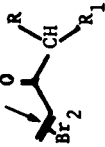
(continued)

Table 3 (cont.)

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
	--	3-3		<u>P. angustum</u>	(43)
	--	3-4	violacene	<u>P. violaceum</u>	(43)
	--	3-5		<u>P. cartilagineum</u>	(43)
	--	3-6		<u>P. cartilagineum</u>	(43)
	--	3-7		<u>P. cartilagineum</u>	(43)
	--	3-8		<u>P. cartilagineum</u>	(43)
	--	3-9	cartilagineal	<u>P. cartilagineum</u>	(43)
	--	3-10		<u>Desmia hornemanni</u>	(43)
	--	3-11		<u>D. hornemanni</u>	(43)
	--	3-12		<u>D. hornemanni</u>	(43)
	--	3-13		<u>D. hornemanni</u>	(43)

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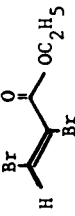
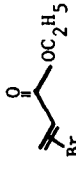
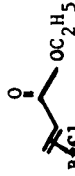
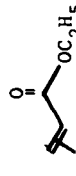
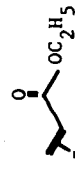
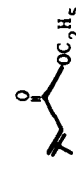
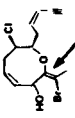
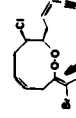
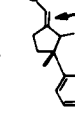
Table 3 (cont.)

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
	--	3-14		<u>D. hornemanni</u>	(43)
	--	3-15		<u>D. hornemanni</u>	(43)
	--	3-16		<u>D. hornemanni</u>	(43)
	--	3-17		<u>D. hornemanni</u>	(43)
Sesquiterpenes					
	R R <sub>1</sub>	3-18	prepacifenol	<u>Laurencia filiformis</u> , <u>L. pacifica</u>	(43)
	-- -Br	3-19	elatol	<u>L. elata</u> , <u>L. obtusa</u>	(43,45)
	-H	3-20		<u>L. obtusa</u>	(45)
Carbonyl-conjugated alkenes					
	-Br	3-21		<u>Asparagopsis taxiformis</u>	(43)
	-Cl	3-22		<u>A. taxiformis</u>	(43)
	-Br	3-23		<u>A. taxiformis</u>	(43)
	-Br	3-24		<u>A. taxiformis</u>	(43)

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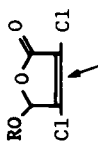
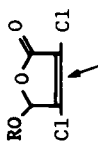
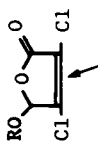
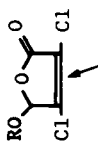
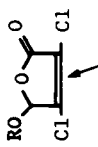




Table 3 (cont.)

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
	--	3-25		<u>A. armata</u>	(46)
	--	3-26		<u>A. armata</u>	(46)
	--	3-27		<u>A. armata</u>	(46)
	--	3-28		<u>A. taxiformis</u>	(46)
	--	3-29		<u>A. taxiformis</u>	(46)
	--	3-30		<u>A. taxiformis</u>	(46)
Epoxide, peroxide, other					
	--	3-31	chondriol	<u>L. sp.</u>	(43)
	--	3-32	rhodophytin	<u>L. sp.</u>	(43)
	--	3-33	laurenisol	<u>L. nipponica</u>	(43)

<sup>a</sup>See Table 5 for other compounds in Rhodophyta and Aplysia species.

Table 4. Haloalkene and cycloalkene, carbonyl- (or -CN) conjugated compounds

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
$\text{CH}_2=\text{CRCl}$	R				
$-\text{CHO}$		4-1	2-propenal, 2-chloro- $\alpha$ -chloroacrolein, 2-chloroacrylaldehyde	Tear gas	(1)
$-\text{CN}$		4-2	2-propenenitrile, 2-chloro- $\alpha$ -chloroacrylonitrile	Polymer and other synthesis	(1)
$-\text{COOH}$		4-3	2-propenoic acid, 3-chloro- $\alpha$ -chloroacrylic acid	Metabolite of 1,3-dichloropropene (compound No. 1-34)	(47)
$-\text{COONa}$		4-4	2-propenoic acid, 3-chloro-, sodium salt (sodium <u>cis</u> -3-chloroacrylate)	Pesticide (defoliant, dessiccant)	(3)
$-\text{H}$		4-5	2-butenic acid, 2,3-dichloro-4-oxo- (mucochloric acid)	(Not found)	(2)
		4-6	bis[3,4-dichloro-2(5H)-furanone], 5,5'-dioxo- (mucochloric anhydride, bis[3,4-dichloro-2(5H)-furanoyl] ether)	Pesticide (fungicide)	(2)
	--	4-7	2-cyclohexen-1-one, 2,3,4,4,5,5,6,6-octachloro- (OCH)	Pesticide (herbicide, fungicide)	(3)
	$\text{R R}_1$				
	$\text{Cl}-\text{Cl}-$	4-8	2,5-cyclohexadiene-1,4-dione, 2,3,5,6-tetrachloro- (chloranil, tetrachloro-p-benzoquinone)	Synthesis of dyes; registered pesticide (fungicide); pH electrodes; vulcanizing agent	(1,2,3)
	$\text{R R}_1$ 	4-9	1,4-naphthalenedione, 2,3-dichloro- (dichlone, 2,3-dichloro-1,4-naphthoquinone)	Organic catalyst; registered pesticide (fungicide for foliage and textiles, seed disinfectant, insecticide)	(1,2,3)

(continued)

Table 4 (cont.)

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
		4-10	mollisin	<u>Mollisia caesia</u> (fungi); fungicidal activity	(48,49)
		4-11	sclerotiorin	<u>Penicillium sclerotiorum</u> , <u>P. multicolor</u> , <u>P. implicatum</u> (fungi)	(48)
		4-12	isobutyl xanthomonadin I	<u>Xanthomonas</u> sp. (bacteria)	(50)
		4-13	phosphoric acid, 2-chloro-3-(diethylamino)-1-methyl-3-oxo-1-propenyl diethyl ester (trans-phosphamidon, phosphamidon, 2-chloro-2-diethylcarbamoyl-1-methylvinyl dimethyl phosphate)	Registered pesticide (insecticide)	(1,2,3)
		4-14	phosphoric acid, 3-chloro-4-methyl-2-oxo-2H-1-benzopyran-7-yl diethyl ester (coumaphos-O-analog, 3-chloro-7-hydroxy-4-methylcoumarin diethyl phosphate)	Drug (ophthalmic anticholinesterase; veterinary -- anthelmintic)	(2)
	(as in 4-14)	4-15	phosphorothioic acid, 0-3-chloro-4-methyl-2-oxo-2H-1-benzopyran-7-yl 0,0-diethyl ester [coumaphos, 0,0-diethyl 0-(3-chloro-7-hydroxy-4-methyl-7-coumarinyl)phosphorothioate]	Veterinary drug (anthelmintic); registered pesticide (insecticide, nematocide)	(1,2,3)
		4-16	androst-4-en-3-one, 17-(acetyloxy)-4-chloro-, (17 $\beta$ ) (4-chlorotestosterone acetate, clostebol acetate)	Drug (anabolic)	(2)

(continued)

Table 4 (cont.)

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
	R R <sub>1</sub>	4-17	pregna-4,6-diene-3,20-dione, 17-(acetyloxy)-6-chloro- (chlormadinone acetate, 6-chloro-6-dehydro-17 $\alpha$ -hydroxyprogesterone acetate)	Drug (progestin; veterinary -- estrus regulator)	(2,7)
	R R <sub>1</sub>	4-18	3'H-cyclopropa[1,2]pregna-1,4,6-triene-3,20-dione, 17-(acetyloxy)-6-chloro-1,2-dihydro- (cyproterone acetate, methylenechlormadinone, SH 714)	Drug (antiandrogen)	(2)
	R R <sub>1</sub> R <sub>2</sub>	4-19	4(1H)-pyridinone, 3,5-diiodo- (lopydone, 3,5-diiodopyridone)	Medical diagnostic (radiopaque medium, bronchographic)	(2)
	R R <sub>1</sub> R <sub>2</sub>	4-20	4(1H)-pyridinone, 1-(2,3-dihydroxypyridyl)-3,5-diiodo- (lopydol)	Medical diagnostic (radiopaque medium, bronchographic)	(2)
	R R <sub>1</sub> R <sub>2</sub>	4-21	1(4H)-pyridineacetic acid, 3,5-diiodo-4-oxo- propyl ester (propyl iodone, propiodone)	Medical diagnostic (radiopaque medium)	(1,2,7)
	R R <sub>1</sub> R <sub>2</sub>	4-22	1(4H)-pyridineacetic acid, 3,5-diiodo-4-oxo- compound with 2,2'-iminodietanol (1:1) [iodopyracet, diiodone, bis(hydroxyethyl)ammonium 3,5-diiodo-4-pyridone-N-acetate]	Medical diagnostic (radiopaque medium, urographic; veterinary -- same)	(1,2,7)
	R R <sub>1</sub> R <sub>2</sub> R <sub>3</sub>	4-23	2,6-pyridine dicarboxylic acid, 1,4-dihydro-3,5-diiodo-1-methyl-4-oxo- sodium salt (sodium iodomethamate, iodoxyl)	Medical diagnostic (radiopaque medium)	(2)
	R R <sub>1</sub> R <sub>2</sub> R <sub>3</sub>	4-24	2,4(1H,3H)-pyrimidinedione, 5-chloro-3-(1,1-dimethylethyl)-6-methyl (terbacil, 3- <u>tert</u> -butyl-5-chloro-6-methyluracil)	Registered pesticide (herbicide)	(2,3)

(continued)

Table 4 (cont.)

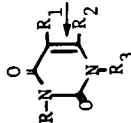
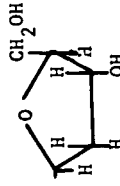
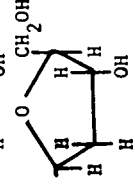
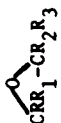
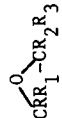
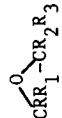
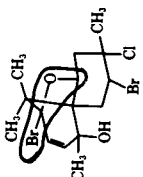
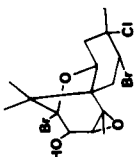
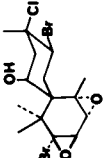
Structure	Substituents			Compound No.	Names	Present or past uses; sources	References
	R	R <sub>1</sub>	R <sub>2</sub> R <sub>3</sub>				
	H-	-F	-H	4-25	2,4-(1H,3H)-pyrimidinedione, 5-fluoro-(5-fluorouracil, 5-FU, FU)	Drug (antineoplastic agent)	(2,7,8)
	H-	-Br	-H	4-26	2,4-(1H,3H)-pyrimidinedione, 5-bromo-(5-bromouracil, 5-BU, BU)	Experimental DNA-incorporatable pyrimidine analog	(51)
	H-	-F	-H	4-27	uridine, 2'-deoxy-5-fluoro- (floxuridine, 5-fluorouracil deoxyriboside, 5-FUDR, FUDR)	Drug (antiviral)	(2)
	H-	-I	-H	4-28	uridine, 2'-deoxy-5-iodo- (idoxuridine, 5-iodouracil deoxyriboside, IDU, IUDR)	Drug (ophthalmic antiviral)	(2)

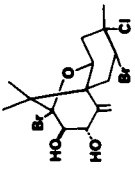
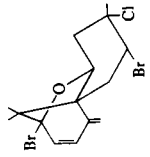
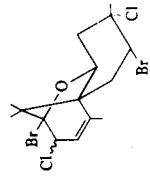
Table 5. Related halogenated compounds

Structure	Substituents			Compound No.	Names	Present or past uses; sources	References
	R	R <sub>1</sub>	R <sub>2</sub> R <sub>3</sub>				
	H	R <sub>1</sub>	R <sub>2</sub> R <sub>3</sub>				
	-H	-H	-H	5-1	oxirane, 1-chloro- (vinyl chloride epoxide, chloroethene oxide, chloroethylene oxide)	Proposed metabolite of chloroethene (vinyl chloride, compound No. 1-1)	(52-54)
	-H	-H	-Cl	5-2	[oxirane, 1,1-dichloro- (vinylidene chloride epoxide)]	Proposed metabolite of 1,1-dichloroethene (compound No. 1-5); not yet synthesized	(52,55, 56)
	-H	-Cl	-H	5-3	oxirane, 1,2-dichloro-, cis-dichloroethylene epoxide	Proposed metabolite of cis-1,2-dichloroethene (compound No. 1-13)	(52,55) (continued)

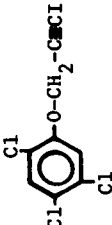
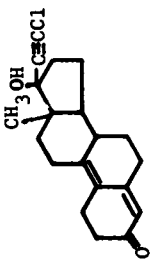
Structure	Substituents			Compound No.	Names	Present or past uses; sources	References
	R	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>			
	(same as 5-3)	-Cl	-Cl	-Cl	5-4 oxirane, 1,2-dichloro-, trans- (trans-1,2-dichloroethylene epoxide)	Proposed metabolite of trans-1,2-dichloroethene (compound No. 1-9)	(52,55)
	-H	-Cl	-Cl	-Cl	5-5 oxirane, trichloro- (trichloroethylene epoxide)	Proposed metabolite of trichloroethene (compound No. 1-17)	(52,55, 57)
	-Cl	-Cl	-Cl	-Cl	5-6 oxirane, tetrachloro- (tetrachloroethylene epoxide)	Proposed metabolite of tetrachloroethene (compound No. 1-21)	(52,55)
	-F	-F	-F	-F	5-7 oxirane, tetrafluoro- (tetrafluoroethylene epoxide, perfluoroethylene oxide, TFEO)	Synthesis of dimers to polymers (Freon E -- coolants for electronic devices)	(1)
	-F	-F	-F	-CF <sub>3</sub>	5-8 oxirane, trifluoro(trifluoromethyl)- (hexafluoropropylene epoxide, perfluoropropylene oxide, HFPO)	Polymer synthesis (lubricating oils and greases)	(1)
	--	--	--	--	5-9 pacifenol	Laurencia pacifica, L. johnstonii, <u>Aplysia californica</u>	(58,59)
	--	--	--	--	5-10 johnstonol	L. pacifica, L. johnstonii, <u>A. californica</u>	(58,60)
	--	--	--	--	5-11 prepacifenol epoxide	L. pacifica, L. johnstonii, <u>A. californica</u>	(43,58)

(continued)

Table 5 (cont.)

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
	--	5-12	johnstondiol	<u>A. californica</u>	(58)
	--	5-13	pacifidiene	<u>A. californica</u> ( <i>in vivo</i> dehydration of pacifenol within the digestive gland)	(61)
	--	5-14		<u>A. californica</u> (secondary product from pacifenol, via pacifidiene, within the digestive gland)	(61)
Aldehydes					
$\text{CH}_2\text{Cl}-\text{CHO}$	--	5-15	acetaldehyde, chloroaldehyde (2-chloroacetaldehyde)	Synthesis; pesticide (fungicide); removal of bark from tree trunks; proposed product of rearrangement of vinyl chloride epoxide (compound No. 5-1)	(1,2,52-54)
$\text{CHCl}_2-\text{CHO}$	--	5-16	acetaldehyde, dichloro-	Synthesis of insecticides; proposed product of rearrangement of both <i>cis</i> - and <i>trans</i> -1,2-dichloroethylene epoxide (compounds No. 5-3 and 5-4)	(1,52)

(continued)

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
$\text{CCl}_3\text{-CHO}$	X --	5-17	acetaldehyde, trichloro- (chloral)	Synthesis of chloral hydrate and DDT; [chloral hydrate is a drug (sedative)]; proposed <u>in vivo</u> product of rearrangement of trichloroethylene epoxide; rearrangement product via Lewis acids	(1,2,7,8,52)
<b>Alcohols</b>					
$\text{CH}_2\text{-CHOH}$	-Cl	5-18	ethanol, 2-chloro- (ethylene chlorohydrin, ethylchlorhydrin, glycol chlorohydrin, 2-chloroethyl alcohol)	Synthesis; solvent; prior treatment of dormant potatoes to sprout after planting	(1,2,62)
<b>Alkynes</b>					
$\text{CX}\equiv\text{CX}$	-Br	5-19	ethanol, 2-bromo- (ethylene bromohydrin)	Synthesis	(1,2)
	-Br	5-20	ethyne, 1,2-dibromo- (dibromoacetylene, dibromoethyne)	Synthesis	(1)
	-I	5-21	ethyne, 1,2-diiodo- (diiodoacetylene)	Synthesis; poison vapor	(1)
$\text{CH}_3\text{-CH}_2\text{-C}\begin{matrix} \text{OH} \\   \\ \text{C} \\   \\ \text{CH}_3 \end{matrix}\text{-C}\equiv\text{CBr}$	--	5-22	1-pentyn-3-ol, 1-bromo-3-methyl- (2-bromoethynyl-2-butanol)	Drug (sedative; compare with compound No. 1-79)	(2)
	--	5-23	benzene, 1,2,4-trichloro-5-((3-iodo-2-propynyl)oxy)- (haloprogin, 2,4,5-trichlorophenyl p-iodopropargyl ether)	Drug (antibacterial)	(2,7,8)
	--	5-24	19-norpregna-4,9-dien-20-yn-3-one, 21-chloro-17-hydroxy-, (17K) (ethyn-erone, MK 665)	Drug (progestin)	(2)

(continued)



Table 5 (cont.)

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
Allylic compounds					
$\text{CH}_2=\text{CRR}_1$	R				
	$\text{R}_1$				
	-H	5-25	1-propene, 3-chloro-1-chloro-2-propene, 2-propenyl chloride, chloroallylene	Polymer and other synthesis	(1,2)
	-H	5-26	1-propene, 3-bromo- (allyl bromide)	Polymer and other synthesis	(1,2)
	-H	5-27	silane, trichloroethenyl- (vinyl trichlorosilane, vinylsilicon trichloride, VTCS)	Synthesis of silicon adhesives	(1)
	-H <sub>3</sub>	5-28	1-propene, 3-chloro-2-methyl- (β-methylallyl chloride, β-chloroisobutylene, MAC)	Polymer and other synthesis; pesticide (fungant)	(1,2)
	---	5-29	benzeneethanamine, α-methyl-N-(2,2,2-trichloroethylidene)- [amphchloral, α-methyl-N-(2,2,2-trichloroethylidene)-phenylethylamine]	Drug (anorexic)	(2)
	X				
	-Cl	5-30	1-propyne, 3-chloro- (propargyl chloride)	Synthesis	(1,2)
	-Br	5-31	1-propyne, 3-bromo- (propargyl bromide)	Synthesis; registered pesticide (soil fungant)	(1,3)
	---	5-32	carbamic acid, (3-chlorophenyl)-, 4-chloro-2-butynyl ester (barban, barbanate, 4-chloro-2-butynyl-3-chlorocarbaniolate)	Registered pesticide (herbicide and plant growth regulator)	(2)

Table 6. Related nonhalogenated species



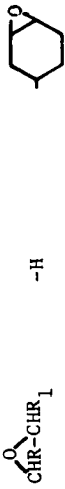













Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
Epoxides and imines 	R				
	R <sub>1</sub>				
	-H	6-1	oxirane, (ethylene oxide, 1,2-epoxyethane, dimethylene oxide, ETO)	Synthesis; registered pesticide (fumigant, insecticide, fungicide); petroleum demulsifier; equipment sterilization; rocket propellant	(1,2,3)
	-H	6-2	oxirane, methyl-1,2-epoxypropane)	Polymer and other synthesis; registered pesticide (fumigant, insecticide, soil sterilant); solvent	(1,2,3)
	-CH <sub>3</sub>				
	-H	6-3	oxirane, chloromethyl- [epichlorohydrin, α-epichlorohydrin, 1-chloro-2,3-epoxypropane, β-chloropropylene oxide, (chloromethyl)ethylene oxide, epi]	Polymer and other synthesis; registered pesticide (fumigant, insecticide); solvent; curing agent for polyene based rubbers; antioxidant in some trichloroethylene preparations	(1,2,3,63)
	-H	6-4	oxirane, ethyl- (1,2-butylene oxide, 1,2-epoxybutane)	Polymer and other synthesis; stabilizer for chlorinated solvents; antioxidant in some trichloroethylene preparations	(1,63)
	-CH <sub>2</sub> -CH <sub>3</sub>				
	-H	6-5	oxirane, methanol (glycidol, 2,3-epoxy-1-propanol, 3-hydroxypropylene oxide, epihydrin alcohol, glycid)	Stabilizer for natural oils and vinyl polymers; demulsifier; dye leveling agent	(1,2)
	-CH <sub>2</sub> OH				
	-H	6-6	2,2'-bioxirane (1,2,3,4-diepoxybutane, butadiene diepoxide, erythritol anhydride)	Curing polymers; cross-linking fibers; prevent microbial spoilage	(2)
	-H	6-7	oxirane, phenyl- (epoxyethylbenzene, styrene oxide, phenylethylene oxide)	Synthesis	(1)
	-H				(continued)

Table 6 (cont.)

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
	R				
	-H	6-8	7-oxabicyclo(4.1.0)heptane, 3-oxiran-yl-(vinylcyclohexene dioxide, vinylcyclohexane dioxide)	Polymer and other synthesis	(1)
	-CH <sub>3</sub>	6-9	oxirane, 1,2-dimethyl- (2,3-butylene oxide, 2,3-epoxybutane)	Synthesis	(1)
	-H	6-10	aziridine (ethyleneimine, azacyclopropane, dimethyleneimine, EI)	Polymer and other synthesis	(1,2)
	-H	6-11	aziridine, 2-methyl- (propyleneimine, 2-methylethyleneimine)	Synthesis	(1)
	-H	6-12	aziridine, 2-ethyl- (2-ethyleneimine)	Synthesis	(1)
	-CH <sub>2</sub> -CH <sub>2</sub> OH	6-13	1-aziridineethanol [N-(2-hydroxyethyl)ethyleneimine]	Synthesis	(1)
	-CH <sub>2</sub> -CH(OH)-CH=CH <sub>2</sub>	6-14	1-aziridineethanol, α-ethenyl- (α-vinyl-1-aziridineethanol, 1-ethyleneimino-2-hydroxy-3-butene)	Experimental neoplastic drug	(2)
Nonconjugated and conjugated alkenes					
	-H	6-15	ethene (ethylene, elayl, bicarburetted hydrogen, olefiant gas)	Polymer and other synthesis; drug (veterinary and human anesthetic); welding and cutting metals; refrigerant; acceleration of fruit ripening	(1,2,3)
	-H	6-16	ethene, methoxy- (methyl vinyl ether, MVE)	Polymer synthesis; plasticizer	(1)
	-H	6-17	ethene, 1,1'-oxybis- (vinyl ether, divinyl ether, divinyl oxide)	Polymer synthesis; drug (anesthetic - vinylcolumbinum, 75% ethyl ether + 25% vinyl ether)	(1,2,4)
	-H	6-18	acetic acid, ethenyl ester (vinyl acetate, vinyl A monomer, 1-acetoxyethylene, VyAc)	Polymer synthesis	(1,2)



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Table 6 (cont.)

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
$\text{CH}_2=\text{CRR}_1$	R				
	$\text{R}_1$				
	-H	6-19	1-propene (propylene, methylethylene)	Polymer and other synthesis; polymer gasoline	(1,2)
	$-\text{CH}_3$				
	-H	6-20	2-propenal (acrolein, acrylaldehyde, acraldehyde, allyl aldehyde)	Polymer and other synthesis; registered pesticide (herbicide, fungicide); tear gas; warning agent in methyl chloride refrigerant	(1,2,3)
	$-\text{CHO}$				
	-H	6-21	2-propenoic acid, (acrylic acid, acroleic acid, vinyl formic acid)	Polymer synthesis	(1,2)
	$-\text{COOH}$				
	-H	6-22	2-propenamide (acrylamide)	Polymer and other synthesis; flocculent; sewage and waste treatment; permanent press fabrics	(1,2)
	$-\text{CONH}_2$				
	-H	6-23	2-propenenitrile (acrylonitrile, vinyl cyanide, cyanoethylene)	Polymer and other synthesis; modifier of natural fiber; registered pesticide (fungant, insecticide)	(1,2,3)
	$-\text{CN}$				
	-H	6-24	1-butene ( $\alpha$ -butylene, ethylethylene)	Polymer and other synthesis	(1,2)
	$-\text{CH}_2-\text{CH}_3$				
	-H	6-25	1,3-butadiene (vinylethylene, bivinylolefin)	Polymer and other synthesis	(1,2)
	$-\text{CH}=\text{CH}_2$				
	-H	6-26	3-butene-2-one (methyl vinyl ketone, methyl vinyl ketone)	Polymer and other synthesis	(1,2)
	$\text{O}$ $-\text{C}-\text{CH}_3$				
	-H	6-27	benzene, ethenyl- (styrene, phenylethylene, vinyl benzene, styrol, cinnamine)	Polymer and other synthesis	(1,2)
					
	-H	6-28	cyclohexene, 4-ethenyl- (4-vinylcyclohexene, 1-vinyl-3-cyclohexene)	Polymer and other synthesis; a butadiene dimer	(1)
					

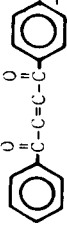



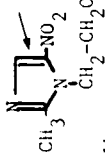
(continued)

Table 6 (cont.)

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
$\text{CH}_2=\text{CRR}_1$	R				
	$\text{R}_1$				
		6-29	7-oxabicyclo(4.1.0)heptane, 3-ethenyl-(vinylcyclohexene monoxide, vinylcyclohexane monoxide)	Polymer and other synthesis	(1)
	$-\text{CH}_3$	6-30	1-propene, 2-methyl- (isobutene)	Polymer and other synthesis	(1)
	$-\text{CH}_2-\text{CH}_3$	6-31	1-butene, 2-methyl-	Synthesis	(1)
	$-\text{CH}=\text{CH}_2$	6-32	1,3-butadiene, 2-methyl- (isoprene)	Polymer and other synthesis; "natural" rubber	(1,2)
	$-\text{CH}_3$	6-33	2-propenoic acid, 2-methyl-, methyl ester (methylmethacrylate, MME)	Polymer synthesis; impregnation of concrete	(1)
	$-\text{C}\equiv\text{CH}$	6-34	1-buten-3-yne, 2-methyl- (isopropenylacetylene)	Synthesis; specialty fuel	(1)
		6-35	benzene, 1-(methylethenyl)- ( $\alpha$ -methylstyrene, 2-phenyl-1-propene, $\alpha$ -methylstyrol)	Polymer synthesis	(1)
	$-\text{CN}$	6-36	2-propenoic acid, 2-cyano-, methyl ester (acrylate, methyl-2-cyanoacrylate)	Polymer and adhesive synthesis; surgical aid (tissue adhesive)	(1,2)
	$-\text{CH}_2-\text{CH}_2\text{CN}$	6-37	1,5-pentanedinitrile, 2-methylene-(methyleneglutaronitrile, 2,4-dicyano-1-butene)	Polymer and other synthesis; acrylonitrile dimer	(1)
$\text{CH}_3-\text{CH}=\text{CRR}_1$	$-\text{CH}_3$	6-38	2-butene (sym-dimethylethylene, $\beta$ -butylene, "high-boiling" butene-2)	Synthesis; cross-linking agent; polymer gasoline	(1,2)
	$-\text{CHO}$	6-39	2-butenal (crotonaldehyde, <u>trans</u> -crotonaldehyde)	Synthesis; solvent; preparation of rubber accelerators; purification of lubricating oils; pesticide (insecticide); tear gas; leather tanning; alcohol denaturant; fuel gas warning agent	(1,2)


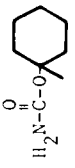
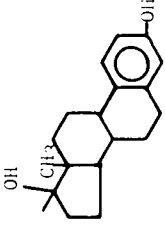
(continued)

Table 6 (cont.)

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
$\text{CH}_3\text{-CH=CRR}_1$	R -H $\text{R}_1$ -COOH	6-40	2-butenoic acid, (crotonic acid, $\beta$ -methylacrylic acid)	Polymer and other synthesis	(1,2)
	-CH <sub>3</sub>	6-41	2-butene, 2-methyl- ( $\beta$ -isoamylene, amylene, trimethylethylene)	Synthesis; drug (dental and surgical anesthetic)	(1,2)
	--	6-42	2-butene-1,4-dione, 1,4-diphenyl- (trans-1,2-dibenzoyl ethylene)	Synthesis; bactericide; enzyme inhibitor	(1)
	--	6-43	cyclopentene	Polymer and other synthesis	(1)
	--	6-44	1,3-cyclopentadiene	Polymer and other synthesis including organometallics	(1,2)
	--	6-45	cyclohexene	Synthesis; catalyst solvent; extraction of oils; suggested stabilizer for high octane gasoline	(1,2)
	--	6-46	1H-imidazole-1-ethanol, 2-methyl-5-nitro- [metronidazole, 1-(2-hydroxyethyl)-2-methyl-5-nitroimidazole]	Drug [antiprotozoal (trichomonas); veterinary -- antiprotozoal, treponemicide]	(2,7,8)
Alkynes					
$\text{CR}_1\text{CR}_2$	-H -CN	6-47	2-propynenitrile (cyanoacetylene)	Synthesis	(64,65)
	-CH <sub>3</sub>	6-48	2-propyne [methylacetylene (stabilized with propadiene)]	Industrial fuel gas for cutting, welding, brazing, heat treating and metallizing	(1)
	-H -CH <sub>2</sub> OH	6-49	2-propyn-1-ol (propargyl alcohol)	Synthesis; pesticide (soil fumigant, insecticide); corrosion inhibitor; solvent stabilizer	(1,2,3)

(continued)

Table 6 (cont.)

Structure	Substituents	Compound No.	Names	Present or past uses; sources	References
$CR_1$	R				
	$R_1$				
$CR_1$	-H	6-50	cyclohexanol, 1-ethynyl-1-cyclohexanol	illizer; prevents hydrogen embrittlement of steel; laboratory reagent	(1,2)
					
	-H	6-51	cyclohexanol, 1-ethynyl-, carbamate (ethinamate, 1-ethynylcyclohexyl carbamate)	Synthesis; stabilization of chlorinated organic compounds; corrosion inhibitor for mineral acids	(1,2)
					
	-H	6-52	19-norpregna-1,3,5(10)-trien-20-yn-3,17-diol, (17 $\alpha$ ) (ethynylestradiol)	Drug (estrogen), veterinary -- (estrogenic hormone therapy)	(1,2)
					

pounds. Also, the forms in which the chemicals are naturally present or are made commercially available may increase or decrease biologic availability and response.

## Sources and Methods

The primary documents searched were *The Condensed Chemical Dictionary* (1), a portion of which was screened because in most cases the structural formula is omitted, *The Merck Index* (2) and the *Pesticide Index* (3). Each reports uses for the compounds. Because an immediately preceding (1, 2) or earlier edition (3) was first used, newly listed compounds could have been omitted. However, all compounds chosen were verified for their current listing and their updated uses. Compounds were also found in other collections, in reviews, and in research reports.

The principle used in deciding on which names to use of the many alternate names listed was, first, the *Chemical Abstracts* name and, second, perhaps more general recognition by alternate names. Other names can be determined by looking at the names of closely related compounds and by referral to the cross indexes in the literature (1-8, 11). Repeatable variations are not routinely shown. The first name is uninverted, as given in the Ninth Collective Index (9CI) of *Chemical Abstracts*. These names are sometimes quite different from those appearing in the Eighth Collective Index (8CI) because of fairly extensive modification of the nomenclature rules in 1972. Generally, in our tables a common name is the first within parentheses. This is an "approved," "official," "generic," "abbreviated chemical," "source" or "trivial name" as defined in *Pharmacological and Chemical Synonyms* (4). Then another chemical name or research code number is indicated. The *Registry of Toxic Effects of Chemical Substances* (5) and *Abstracts on Health Effects of Environmental Pollutants: Chemical Index Guide* (6) assisted in identifying additional names.

The first name used in the above collections has been called the "prime," "index" or "title name" and it varies considerably from one collection to another. The following guide should assist in determining a first name used elsewhere. Equivalent nomenclature forms are: -ene and -ylene; ethenyl and vinyl; chloro-, chlor- and clor-; di- and bi-;  $\alpha$ ,  $\beta$  . . . and 1,2 . . .; inverted forms such as bromochloro- and chlorobromo-; abbreviated names as in dibromodiodoethene (which is ambiguous) and 1,2-dibromo-1,2-diiodoethene, and both CFE and CTFE for chlorotrifluoroethene; and other examples of earlier *Chemical Abstracts* and

other nomenclature systems. Frankly misleading names remain popular. Some have been based upon a route of synthesis, for example, acetylene dichloride for 1,2-dichloroethene, and abbreviation, for example, both ethylene chloride and ethylene dichloride (which suggest an alkene) for 1,2-dichloroethane. The stereochemical isomers or mixtures of isomers of the compounds are not uniformly noted in our tables and these are not standardized to the latest systems because of the complexity of the subject. However, the existence of multiple isomers should be kept in mind and it is, in fact quite common. Some compounds have two or even three stereochemical sites, for example, compounds 1-68 and 1-69 have three such sites.

A compound may no longer actually be used as indicated, and probably not all uses have been identified. It is essentially impossible to sort these and be completely up to date. Vinyl chloride, for example, should no longer be used as a propellant or refrigerant since it has been banned in these uses. In the case of pesticides, those currently registered, even for very limited uses, are indicated as such. Some of these might be under reconsideration. Drugs included in *APhA Drug Names* (7) and *Physician's Desk Reference* (8) are indicated. A few of the compounds are included here because of their close structural relationship to other listed compounds despite absence of an indicated use or source.

The organization of the six tables is shown below and the number of compounds in each section is shown in brackets. In Tables 1-6, arrows are sometimes used to designate a haloethylene substructure not immediately apparent. Some of the compounds and groups have been considered at this conference either in depth or for more compounds than shown within groups here.

Table 1 (haloalkenes) includes: ethenes [31], propenes [8], butenes [11], organophosphate and sulfonyl compounds [9], thiocarbamates [3], pyrethroids [7], barbiturates [4], amino acids and fatty acids [4], and other compounds and isosteres [7].

Table 2 (halocycloalkenes and ring-conjugated haloalkenes) includes: pentadienes and isosteres [15], methanocyclohexenes [13], and di- and triphenylethylenes [5].

Table 3 includes: haloalkene and halocycloalkene compounds from *Rhodophyta* species and in a feeder species; monoterpenes [17], sesquiterpenes [3], carbonyl-conjugated alkenes [10], and an epoxide, peroxides, and other compounds [3].

Table 4 lists: haloalkene and cycloalkene, carbonyl- (or -CN) conjugated compounds [28].

Table 5 (related halogenated compounds) includes: epoxides [14], aldehydes [3], alcohols [2],



alkynes [5], allylic compounds [5], and allylic alkynes [3].

Table 6 (related nonhalogenated compounds) includes: epoxides and imines [14], nonconjugated and conjugated alkenes [32], and alkynes [6].

We are pleased to acknowledge the help of Mr. Ralph Hester in assembling some of the information in this report.

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