Haloethylenic-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 haloethylenic 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 knowing 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 haloethylenic 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 halalkanes, for example, are not here because of their large number, despite the knowledge that some are either metabolized or nonbiologically converted to halokalenes.

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 alklenes); 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-

*Office of Health Hazard Assessment, National Institute of Environmental Health Sciences, National Institutes of Health, P. O. Box 12233, Research Triangle Park, North Carolina 27709.
| Structure   | Substituents | Compound No. | Names                                                                 | Present or past uses; sources | References |
|------------|--------------|--------------|----------------------------------------------------------------------|-------------------------------|------------|
| Ethenes    | X            | 1-1          | ethene, chloro- (vinyl chloride, vinyl chloride monomer, chloroethylene, VC, VCM) | Polymer and other synthesis; propellant; refrigerant | (1,2,9)    |
|            | -Cl          | 1-2          | ethene, bromo- (vinyl bromide)                                       | Polymer and other synthesis; flame retardant | (1)        |
|            | -Br          | 1-3          | ethene, fluoro- (vinyl fluoride)                                     | Polymer and other synthesis   | (1)        |
|            | -I           | 1-4          | ethene, iodo- (vinyl iodide)                                         | (Not found)                   | (10)       |
| CH₂=CHX    | -Cl          | 1-5          | ethene, 1,1-dichloro- (vinylidine chloride, 1,1-dichloroethylene, asym-dichloroethylene) | Polymer and other synthesis   | (1,2,9)    |
|            | -Br, -F or -I| 1-6          | (Named as in 1-5)                                                    | (Br and F) Polymer and other synthesis; (1) not found | (1,10,11)  |
| CH₂=CH₂    | -Cl          | 1-7          | ethene, 1,2-dichloro-, (trans-) (sym-trans-dichloroethylene, trans-acetylene dichloride) | Synthesis; solvent (trans- and cis, trans- mixture used more than cis-); retarding fermentation | (1,2,12)   |
|            | -Br, -F or -I| 1-8          | (Named as in 1-9)                                                    | (Not found)                   | (2,10,11)  |
| CH=CH      | -Cl          | 1-9          | ethene, 1,2-dichloro-, (cis-) (named as in 1-9, but cis-)             | Synthesis                     | (1)        |
|            | -Br, -F or -I| 1-10         | (As in 1-9, but cis-)                                                | (Not found)                   | (10,11)    |
| CHX=CH₂    | -Cl          | 1-11         | ethene, 1,2-dichloro-, (trans-) (named as in 1-9, but cis-)           | Synthesis                     | (1)        |
|            | -Br, -F or -I| 1-12         | (As in 1-9, but cis-)                                                | (Not found)                   | (10,11)    |
|            | -Cl          | 1-13         | ethene, trichloro- (1,1,2-trichloroethylene, acetylene trichloride, ethylene trichloride, ethynyl trichloride, tri, TCE) | Synthesis; solvent; registered pesticide (fumigant); drug (analgesic, anesthetic); | (1,2,3,7)  |

(continued)
| Structure  | Substituents | Compound No. | Names                                      | Present or past uses; sources                          | References |
|-----------|--------------|--------------|--------------------------------------------|-------------------------------------------------------|------------|
| CHX=CH2   | -Br, -F or -I| 1-18         | (Named as in 1-17)                         | solvent dyeing; cleaning and drying metal; flushing liquid oxygen | (10,11)   |
| CX2=CH2   | -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         | [As 1-21 and also: (F) TFE, (I) ethylene periodide, difluoroform, iodo-ethylenes] | (Br and F) Polymer and other synthesis; (I) drug (surgical dusting powder, antiseptic ointment); pesticide (fungicide) | (1,2,3)   |
| CH2=CBrCl | --           | 1-25         | ethene, 1-bromo-1-chloro-                  | Fire retardant                                         | (13)       |
| CHCl=CF2  | --           | 1-26         | ethene, 1-chloro-2,2-difluoro-             | Polymer synthesis; metabolite of halothane (CHBrCl-CF2) | (14)       |
| CClF=CF2  | --           | 1-27         | ethene, chlorotrifuoro- (monochlorotrifuoroethylene, trifluorovinyl chloride, CFE, CTFE) | Polymer synthesis                                     | (1)        |
| CBrF=CF2  | --           | 1-28         | ethene, bromotrifuoro- (BFE)               | Polymer synthesis                                     | (1)        |
| CBrCl=CF2 | --           | 1-29         | ethene, 1-bromo-1-chloro-2,2-difluoro-     | Metabolite of halothane (CHBrCl-CF2)                  | (14)       |
| CCl2=CF2  | --           | 1-30         | ethene, 1,1-dichloro-2,2-difluoro-         | Polymer and other synthesis                            | (15)       |
| CBrI=CBrI | --           | 1-31         | ethene, 1,2-dibromo-1,2-diiodo- (sym-dibromodiiodoethylene) | Synthesis                                             | (1)        |

(continued)
| Structure | Substituents | Compound No. | Names                                                                 | Present or past uses; sources | References |
|-----------|-------------|--------------|----------------------------------------------------------------------|-------------------------------|------------|
| Propenes  | R R₁ X      |              |                                                                      |                               |            |
| RCH=CHCl  | Cl⁻         | 1-32         | 1-propene, 1-chloro- (propenyl chloride)                             | (Not found)                   | (5)        |
|           | CH₂OH⁻      | 1-33         | 1-propene-3-ol, 1-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)       |
| RCH=CHCl  | CH₂Cl⁻      | 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 chloropirin -- soil fumigant and nematocide) | (1,2,3,17) |
|           | CH₂Br⁻      | 1-35         | 1-propene, 3-bromo-1-chloro- (CBP, CBP-55)                           | Pesticide (soil fumigant)     | (3)        |
| RCC1=CH₂  | CH₃⁻        | 1-36         | propene, 2-chloro- (isopropenyl chloride)                             | Polymer and other synthesis   | (1,5)      |
|           | CH₂Cl⁻      | 1-37         | 1-propene, 2,3-dichloro-                                              | Contaminant of DD (see compound No. 1-34) | (18)       |
| CX₂=CX₂  | -Cl         | 1-38         | propene, 1,1,2,3,3,3-hexachloro- (perchloropropylene)                | Solvent; plasticizer; hydraulic fluid | (1)        |
|           | -F          | 1-39         | propene, 1,1,2,3,3,3-hexafluoro- (perfluoropropylene, HFP)            | Polymer synthesis             | (1)        |
| Butenes   |             |              |                                                                      |                               |            |
| RCR₁=CHX  | CH₃⁻ -CH₃ -Cl | 1-40         | 1-propene, 1-chloro-2-methyl- (chloroisobutylene, α,β-dimethylvinyl chloride, isocretyl chloride) | Synthesis                     | (2)        |

(continued)
| Structure     | Substituents | Compound No. | Names                                      | Present or past uses; sources                  | References |
|---------------|--------------|--------------|--------------------------------------------|------------------------------------------------|------------|
| RCR<sub>1</sub>-CH<sub>2</sub>Cl-CHCl<sub>2</sub>- | CH<sub>2</sub>Cl-CHCl<sub>2</sub>- | -H | -Cl | 1-41 | 1-butene, 1,3,4-trichloro- | Contaminant of vinyl chloride via oxychlorination synthesis | (19) |
| RCX=CH<sub>2</sub> | CH<sub>2</sub>Cl-CHCl<sub>2</sub>- | -- | -Cl | 1-42 | 1-butene, 2,3,4-trichloro- | Contaminant of vinyl chloride via oxychlorination synthesis | (19) |
| CH<sub>2</sub>=CH<sub>2</sub>- | CH<sub>2</sub>=CH<sub>2</sub>- | -- | -Cl | 1-43 | 1,3-butadiene, 2-chloro- (chloroprene, 2-chlorobutadiene) | Synthesis of polychloroprene (neoprene) | (1) |
| CH<sub>3</sub>-CC1=CH-CH<sub>2</sub>Cl | -- | -- | -- | 1-44 | 2-butene, 1,3-dichloro- | Contaminant of chloroprene via acetylene synthesis | (1,20) |
| CH<sub>2</sub>Cl-CH=CC1-CH<sub>2</sub>Cl | -- | -- | -- | 1-45 | 2-butene, 1,2,4-trichloro- | Contaminant of vinyl chloride via oxychlorination synthesis | (19) |
| CF<sub>3</sub>- | CF<sub>3</sub>- | -- | -- | 1-46 | 1-propene, 1,1,3,3,3-pentafluoro-2-trifluoromethyl- (octafluorobutene, perfluorobutene, PFIB) | Most toxic fluoroalkene tested to date | (21) |
| CF<sub>3</sub>- | CF<sub>3</sub>- | -- | -- | 1-47 | 1,3-butadiene, 1,1,2,3,4,4-hexachloro- (hexachlorobutadiene, perchlorobutadiene, HCBD, C-46) | Solvent; heat transfer liquid; transformer and hydraulic fluid; by-product of hexachlorobenzene synthesis | (1,22) |
| RCX=CR<sub>1</sub>X | CH<sub>2</sub>OH- | =CH<sub>2</sub>OH | -Br | 1-48 | 2-butene-1,4-diol, 2,3-dibromo- (dibromobutenediol) | Flame retardant | (13) |
| CF<sub>3</sub>- | CF<sub>3</sub>- | -Cl | 1-49 | 2-butene, 2,3-dichloro-1,1,1,4,4,4-hexafluoro- (DCHFB, HFCB) | A toxic impurity of halothane (CHBrCl-CF<sub>3</sub>) | (21) |
| CF<sub>3</sub>- | CF<sub>3</sub>- | -F | 1-50 | 2-butene, 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 | R₁ | | | | |
| (R)₂'O-OR₁ | C₂H₅O⁻ | -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) |
| | C₂H₅O⁻ | -C=CHCl | 1-52 | phosphoric acid, 2-chloro-1-(2,4-dichlorophenyl)ethenyl diethyl ester (chlofenvinfos, chlofenvinfos, as in 1-51) | Registered pesticide (insecticide) | (2,3) |
| | CH₃O⁻ | -C=CHCl | 1-53 | phosphoric acid, 2-chloro-1-(2,4,5-trichlorophenyl)ethenyl dimethyl ester (stirosol, tetrachlorvinfos, CVMP, as in 1-51) | Registered pesticide (insecticide) | (2,3) |
| | C₂H₅O⁻ | -CH₂-CHCl-O-CH=CCl₂ | 1-54 | phosphoric acid, 1-(2-chloroethoxy)-2,2-dichloroethenyl diethyl ester (phosphinon, as in 1-51) | Pesticide (insecticide) | (3) |
| | CH₃O⁻ | -CH=CCl₂ | 1-55 | phosphoric acid, 2,2-dichloroethenyl dimethyl ester (dichlorvos, chlofenvinfos, DDVP, as in 1-51) | Veterinary drug (anthelmintic, insecticide); registered pesticide (insecticide, fumigant) | (1,2,3) |
| | CH₂Cl-CH₂-O-P-O-CH=CCl₂ | -- | 1-56 | phosphoric acid, 2-chloroethyl 2,2-dichloroethenyl) ethyl ester (as in 1-51) | Pesticide (insecticide) | (3) |
| | (C₂H₅O)₂-P-O-C=CHCl | -- | 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-CCl=CHCl | CH₃⁻ | -- | 1-58 | ethene, 1,2-dichloro-1-methylsulfonyl)- [1,2-dichloro-1-(methylsulfonyl)ethyline, D-113] | Pesticide (fungicide) | (5) |

(continued)
Table 1 (cont.)

| Structure | Substituents | Compound No. | Names | Present or past uses; sources | References |
|-----------|--------------|--------------|-------|-------------------------------|------------|
| R-S-CCl=CHCl | C₄H₉⁻ | -- | 1-59 | butane, 1-((1,2-dichloroethenyl)sulfonyl)- (1,2-dichloro-1-butylsulfonyl-ethylene, D-121) | Pesticide (fungicide) | (3) |
| S | (R)₂-N-C-S-CH₂R₁ | C₂H₅⁻ | -CCl=CH₂ | 1-60 | carbamothioic acid, diethyl-, 2-chloro-2-propenyl ester (sulfallate, thioallate, 2-chloroallyl N,N-diethyl-dithiocarbamate, CDEC) | Registered pesticide (herbicide) | (1,3) |
| S | (R)₂-N-C-S-CH₂R₁ | (CH₃)₂CH⁻ | -CCl=CHCl | 1-61 | carbamothioic acid, bis(1-methylethyl)- S-(2,3-dichloro-2-propenyl) ester [diallate, S-(2,3-dichloroallyl)diisopropylthiocarbamate, DATC, 2,3-DCOT] | Registered pesticide (herbicide) | (1,2,3) |
| S | (R)₂-N-C-S-CH₂R₁ | (CH₃)₂CH⁻ | -CCl=CCl₂ | 1-62 | carbamothioic acid, bis(1-methylethyl)- S-(2,3,3-trichloro-2-propenyl) ester [triadate, S-(2,3,3-trichloroallyl) diisopropylthiocarbamate] | Registered pesticide (herbicide) | (1,3) |

Pyrethroids

| Structure | Substituents | Compound No. | Names | Present or past uses; sources | References |
|-----------|--------------|--------------|-------|-------------------------------|------------|
| R | CH=CHCl | 1-63 | cyclopropane carboxylic acid, 3-(2-chloroethenyl)-2,2-dimethyl-, (5-(phenylmethyl)-3-furanyl)methyl ester | Pesticide (insecticide) | (23,24) |
| R | CH=CCl₂ | 1-64 | cyclopropane carboxylic acid, 3-(2,2-dichloroethenyl)2,2-dimethyl-, (5-(phenylmethyl)-3-furanyl)methyl ester | Pesticide (insecticide) | (23-25) |
| R | CH=CB₉₂ | 1-65 | cyclopropane carboxylic acid, 3-(2,2-dibromoethenyl)2,2-dimethyl-, (5-(phenylmethyl)-3-furanyl)methyl ester (bromethrin) | Pesticide (insecticide) | (23-26) |
| R | CH=CF₂ | 1-66 | cyclopropane carboxylic acid, 3-(2,2-difluoro ethenyl)-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 |
|-----------|--------------|--------------|-------|-------------------------------|------------|
| ![Structure](image) | -CH₂ - CH=CCl₂ | 1-67 | cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, 3-(phenoxyphenyl)methyl ester (permethrin, NRDC 143, dl-cis, trans; bio-permethrin, NRDC 147, d-trans) | Pesticide (insecticide) | (24,25, 28,29) |
| ![Structure](image) | CN | 1-68 | cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester (NRDC 149, 1RS,3RS,αRS) | Pesticide (insecticide) | (24,25) |
| ![Structure](image) | CN | 1-69 | cyclopropanecarboxylic acid, 3-(2,2-dibromoethyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester [decamethrin, NRDC 161, [S]-αcyano-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) |
| ![Structure](image) | -CH₂ - CH=CH₂ | 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) |
| ![Structure](image) | CH₃ | 1-71 | 2,4,6(1H,3H,5H)-pyrimidinetrione, 5-(2-bromo-2-propenyl)-5-(1-methylpropyl)- [butallylional, sombutal, 5-(2-bromoallyl)-5-sec-butylbarbituric acid] | Drug (hypnotic) | (2,33) |
| ![Structure](image) | CH₃ | 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) |
| ![Structure](image) | CH(CH₃)₂ | 1-73 | 2,4,6(1H,3H,5H)-pyrimidinetrione, 5-(2-bromo-2-propenyl)-5-(1-methylethyl)- [propallylional, 5-(2-bromoallyl)-5-isopropylbarbituric acid] | Drug (hypnotic, sedative) | (2) |

Environmental Health Perspectives
### Table 1 (cont.)

| Structure | Substituents | Compound No. | Names | Present or past uses; sources | References |
|-----------|--------------|---------------|-------|-------------------------------|------------|
| Amino acids and fatty acids | | | | | |
| HOOCC=CH-CH₂-SR | -CCl=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) |
| | -CCl=CCl-S-CH₂-CH₂-COOH | | | | |
| | -CCl=CCl₂ | 1-75 | L-cysteine, S-(1,2,2-trichloroethenyl)- | In vitro reaction product of tetrachloroethene with cysteine | (34,35) |
| | CH₃-(CH₂)₇-Cl=Cl-(CH₂)₇-COOC₂H₅ | | 1-77 | 13-docosenoic acid, 13,14-diodo-, ethyl ester (iodobrassid, ethyl diodobrassidate) | Drug (iodine source) | (2) |
| Others and isosteres | | | | | |
| Cl₂AsCH=CHCl | -- | 1-78 | arseneous dichloride, (2-chloroethenyl)- [lewisite, dichloro(2-chlorovinyl)arsine, chlorovinyl arsine dichloride] | Poison gas | (1,2) |
| CH₃-CH₂-C=CH=CHCl | -- | 1-79 | 1-penten-4-yn-3-ol, 1-chloro-3-ethyl- (ethchlorvynol, ethyl β-chlorovinyl ethynyl carbinol) | Drug (hypnotic, sedative) | (1,2,7,8) |
| [CH₂-C=CH=CHCl] | | | | | |
| Cl⁻ | -- | 1-80 | 3,5,7-triaza-1-azoniatricyclo(3.3.1.1.- (3,7))decane, 1-(3-chloro-2-propenyl)-, chloride [1-(3-chloroallyl)-3,5,7- triaza-1-azoniaadamantane chloride, N-(3-chloroallyl)hexamethylen chloride] | Bactericide (used in latexes, paint, floor polish, joint cement, adhesives, inks, starches, etc.) | (1,2) |
| (CH₃)₂N=N-C-CH₂-S-CH=CCl-CH₃ | -- | 1-81 | 4-thia-1-azabicyclo(3.2.0)heptane-2-carboxylic acid, 6(((3-chloro-2-buteny1)thio)acetyl)amino)-3,3-dimethyl- 7-oxo, monopotassium salt, (2S-(2S,6R) (penicillin S potassium) | Drug (antibiotic) | (2) |
| | | | | | |
| | | | | | |
| NH₂ | R | 1-82 | Experimental irreversible inhibitor of flavin-linked monamine oxidases | | (37) |
### Table 1 (cont.)

| Structure | Substituents | Compound No. | Names | Present or past uses; sources | References |
|-----------|--------------|--------------|-------|-------------------------------|------------|
| ![Structure](image) | H- | 1-83 | benzenecarboxylozoneyl chloride, N-(2,4,6-trichlorophenyl)- [benzoyl chloride (2,4,6-trichlorophenyl)hydrazone] | Pesticide (acaricide) | (18) |
| ![Structure](image) | CH₃- | 1-84 | benzenecarboxylozoneyl chloride, 4-methyl-N-phenyl- (p-tolyl chloride phenyhydrazone) | Experimental drug | (38) |

### Table 2. Halocycloalkenes and ring-conjugated haloalkenes

| Structure | Substituents | Compound No. | Names | Present or past uses; sources | References |
|-----------|--------------|--------------|-------|-------------------------------|------------|
| **Pentadienes and Isosteres** | 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) |
| ![Structure](image) | -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) |
| ![Structure](image) | -- | 2-3 | 1H-pyrole, 3-chloro-4-(3-chloro-2-nitrophene)- (pyroline) | Drug (antifungal) | (2) |
| ![Structure](image) | -- | 2-4 | 1H-pyrole, 2,3,4,5-tetraiodo- (iodopyrole) | Drug (topical antiseptic; veterinary -- topical antiseptic in female reproductive tract) | (2) |
| ![Structure](image) | -H | 2-5 | ergoline-8-carboxamide, 2-bromo-9,10-didehydro-N,N-diethyl-6-methyl, (8β) (bromo-LSD, D-2-bromolysergic acid diethylamide, bromolysergide) | Experimental serotonin antagonist | (2,39) |
| ![Structure](image) | -CH₃ | 2-6 | ergoline-8-carboxamide, 2-bromo-9,10-didehydro-N,N-diethyl-1,6-dimethyl- (8β) | Experimental psychotropic drug | (39) (continued) |
| Structure                                                                 | Substituents | Compound No. | Names                                                                 | Present or past uses; sources | References |
|--------------------------------------------------------------------------|--------------|--------------|----------------------------------------------------------------------|-------------------------------|------------|
| R                                                                        |              | 2-7          | 1,2-ethanediame, N-((5-chloro-2-thienyl)methyl)-N,N'-dimethyl-N-2-pyridinyl- (chlorothen, chloropyrile, chloromethapryline) | Drug (antihistaminic)          | (2)        |
|                                                                          |              | 2-8          |                                                                       | Experimental antihypertensive agent | (40)       |
|                                                                          |              | 2-9          | thiophene, tetrachloro- (perchlorothiophene, TCTP, TD-183)            | Registered pesticide            | (1,3)      |
|                                                                          |              | 2-10         | 5-isoxazoleacetic acid, α-amino-3-chloro-4,5-dihydro-                | Experimental antineo-           | (41)       |
|                                                                          |              |              |                                                                      | plastic drug; Streptomyces      |            |
|                                                                          |              |              |                                                                      | aviges (fungi)                 |            |
|                                                                          |              | 2-11         | 1H-purine-2,6-dione, 8-chloro-3,7-dihydro-1,3-dimethyl-, compound with 2-(diphenylimethoxy)-N,N-dimethylethlanmine (1:1) (dimenhydrinate, compounds 2-11 to 2-13 have also been named as the 8-chlorothophylene compound with the positively charged molecule) | Drug (human and veterinary 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-dimethylethlanmine (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-(diphenylimethoxy)-1-methylpiperidine (1:1) (piprinhydrinate, also named as in 2-11) | Drug (antihistaminic, antiemetic) | (2)        |

(continued)
Table 2 (cont.)

| Structure | Substituents | Compound No. | Names | Present or past uses; sources | References |
|-----------|--------------|--------------|-------|--------------------------------|------------|
| [Image] | [Image] | 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-bromotheophylline compound with the positively charged molecule) | Drug (diuretic) | (2,8) |
| [Image] | [Image] | 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) |
| [Image] | [Image] | 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) |
| [Image] | [Image] | 2-17 | 2,5-methano-2H-indeno(1,2-b)oxirene, 1a,2,3,4,5,6a,7,7-octachloro-1a,1b,5,6,6a-hexahydro- (oxychlordane, chlordane epoxide) | Metabolite of chlordane (compound No. 2-16) | (42) |
| [Image] | [Image] | 2-18 | 4,7-methano-1H-indene, 1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro-heptachlor, 3-chlorochlordene | Registered pesticide (insecticide) | (1,2,3) |
| [Image] | [Image] | 2-19 | 2,5-methano-2H-indeno(1,2-b)oxirene, 2,3,4,5,6,7,7-heptachloro-1a,1b,5,6,6a-hexahydro- (heptachlor epoxide) | Metabolite of heptachlor (compound No. 2-18); insecticide activity | (1,3) |
| [Image] | [Image] | 2-20 | 4,7-methano-1H-indene, 4,5,6,7,8,8-hexachloro-3a,4,7,7a-tetrahydro-(chlordene) | Synthesis of chlordane | (3) |
| [Image] | [Image] | 2-21 | 1,4:5,6-dimethanonaphthalene, 1,2,3,4,-10-hexachloro-1,4,4a,5,8,8a-hexahydro- (1a, 6a, 4a, 5a, 8a, 8aβ) (aldrin, HHDN) | Registered pesticide (insecticide) | (1,2,3) |

(continued)
| Structure | Substituents | Compound No. | Names | Present or past uses; sources | References |
|-----------|-------------|--------------|-------|-------------------------------|------------|
| R | (as in 2-21) | 2-22 | 1,4:5,8-dimethanaphthalene, 1,2,3,4,5,8-hexachloro-1,4,4a,5,8a-hexahydro- (1α,2α,4α,5β,8β,8aα) - (isodrin, the 5β,8β isomer of compound No. 2-21) | Pesticide (insecticide) | (1,2,3) |
| | (as in 2-23) | 2-23 | 2,7:3,6-dimethanaphthal(2,3-b)oxirene, 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,- 7,7a-octahydro-, (1α,2α,2α,2aα,3β,6β,6αβ,7β,7aα) - (dieldrin, aldrin epoxide, HEOD) | Veterinary drug and registered pesticide (insecticide) | (1,2,3) |
| | | 2-24 | 2,7:3,6-dimethanaphthal(2,3-b)oxirene, 3,4,5,6,9-hexachloro-1a,2,2a,3,6,6a,- 7,7a-octahydro-, (1α,2α,2α,2aα,3β,6β,6αβ,7β,7aα) - (endrin, the 2α,3α,6αβ,7β,7aα 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, chloethione) | 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-hexa- hydro- (isobenzan) | Registered pesticide (insecticide) | (1,2,3) |
| | | 2-27 | 4,7-methanoisobenzofuran-1,3-dione, 4,- 5,6,7,8-hexachloro-3a,4,7,7a-tetra- hydro- (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)
Table 2 (cont.)

| Structure | Substituents | Compound No. | Names                                                                 | Present or past uses; references |
|-----------|--------------|--------------|----------------------------------------------------------------------|----------------------------------|
| Di- and triphenylethenes                                                                                           |
| ![Structure](image) | R R1 R2 X | 2-29 | benzene, 1,1'-((dichloroethenylidene)-bis(4-chloro)- [DDE, 1,1-dichloro-2,2-di(p-chlorophenyl)ethylene] | Contaminant and metabolite of DDT (1,3) |
| (C\textsubscript{2}H\textsubscript{5})N-CH\textsubscript{2}-CH\textsubscript{2}-O- | -H | 2-30 | Ethanamine, 2-(4-(2-chloro-1,2-diphenylethynyl)phenoxy)-N,N-diethyl- (clomiphene, chloramphene) | Drug [gonad stimulation (ovulation induction)] (2,7,8,33) |
| CH\textsubscript{3}O- | -OCH\textsubscript{3} | 2-31 | Benzene, 1,1',1"-(1-chloro-1-ethenyl-2-ylidene)tris(4-methoxy)- [chlorotriamine, chlorotris(p-methoxyphenyl) ethylene] | Drug (estrogen) (2,7,8,33) |
| CH\textsubscript{3}-C-O- | -O-C-CH\textsubscript{3} | 2-32 | Phenol, 4,4'-(\textalpha-bromobenzylidine)methylene)di-, diacate (8CI) 4,4'-(\textbeta-bromostyrilidine)diphenol diacate | Drug (estrogen) (2) |
| C\textsubscript{2}H\textsubscript{5}- | -H | 2-33 | Benzene, 1-(2-bromo-1,2-diphenylethenyl)-4-ethyl- (Braparestrrol) 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)\textsuperscript{a}

| Structure | Substituents | Compound No. | Names                                                                 | Present or past uses; references |
|-----------|--------------|--------------|----------------------------------------------------------------------|----------------------------------|
| Monoterpenes                                                                                                           |
| ![Structure](image) | -- | 3-1 | Plocamium cartilagine-neum; A. californica | (43,44) |
| ![Structure](image) | -- | 3-2 | Plocamium sp.; A. californica | (43,44) |

(continued)
| Structure | Substituents | Compound No. | Names         | Present or past uses; sources | References |
|-----------|--------------|--------------|---------------|-------------------------------|------------|
|           |              | 3-3          |               |                               | (43)       |
|           |              | 3-4          | violacene     |                               | (43)       |
|           |              | 3-5          |               |                               | (43)       |
|           |              | 3-6          |               |                               | (43)       |
|           |              | 3-7          |               |                               | (43)       |
|           |              | 3-8          |               |                               | (43)       |
|           |              | 3-9          | cartilagineal |                               | (43)       |
|           |              | 3-10         |               | Desmia hornemanni             | (43)       |
|           |              | 3-11         |               | D. hornemanni                 | (43)       |
|           |              | 3-12         |               | D. hornemanni                 | (43)       |
|           |              | 3-13         |               | D. hornemanni                 | (43)       |

(continued)
| Structure | Substituents | Compound No. | Names | Present or past uses; sources | References |
|-----------|-------------|--------------|-------|-----------------------------|------------|
|           | --          | 3-14         |       | D. hornermanni              | (43)       |
|           | --          | 3-15         |       | D. hornermanni              | (43)       |
|           | --          | 3-16         |       | D. hornermanni              | (43)       |
|           | --          | 3-17         |       | D. hornermanni              | (43)       |
| Sesquiterpenes | --          |              |       |                              |            |
|           | --          | 3-18 prepacifenol |       | Laurencia filiformis, L. pacifica | (43)       |
|           | --          | 3-19 elatol  |       | L. elata, L. obtusa         | (43,45)    |
|           | --          | 3-20         |       | L. obtusa                   | (45)       |
| Carbonyl-conjugated alkenes | --          | 3-21         |       | Asparagopsis taxiformis      | (43)       |
|           | --          | 3-22         |       | A. taxiformis                | (43)       |
|           | --          | 3-23         |       | A. taxiformis                | (43)       |
|           | --          | 3-24         |       | A. taxiformis                | (43)       |

(continued)
| Structure | Substituents | Compound No. | Names   | Present or past uses; sources | References |
|-----------|-------------|--------------|---------|-------------------------------|------------|
| ![Structure 1](image1) | --          | 3-25         |         | A. armata                      | (46)       |
| ![Structure 2](image2) | --          | 3-26         |         | A. armata                      | (46)       |
| ![Structure 3](image3) | --          | 3-27         |         | A. armata                      | (46)       |
| ![Structure 4](image4) | --          | 3-28         |         | A. taxiformis                  | (46)       |
| ![Structure 5](image5) | --          | 3-29         |         | A. taxiformis                  | (46)       |
| ![Structure 6](image6) | --          | 3-30         |         | A. taxiformis                  | (46)       |
| Epoxide, peroxide, other | | | | | |
| ![Structure 7](image7) | --          | 3-31         | chondriol | L. sp.                        | (43)       |
| ![Structure 8](image8) | --          | 3-32         | rhodophytin | L. sp.                       | (43)       |
| ![Structure 9](image9) | --          | 3-33         | laurenisol | L. nipponica               | (43)       |

*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 |
|----------------------------|--------------|--------------|----------------------------------------------------------------------|-------------------------------|------------|
| R                          |              |              |                                                                      |                                |            |
| CH₂=CRCl                   | -CHO         | 4-1          | 2-propanal, 2-chloro- (α-chloroacrolein, 2-chloroacrylaldehyde)      | Tear gas                      | (1)        |
|                            | -CN          | 4-2          | 2-propenenitrile, 2-chloro- (α-chloroacrylonitrile)                  | Polymer and other synthesis   | (1)        |
| CHCl=CHR                   | -COOH        | 4-3          | 2-propenoic acid, 3-chloro- (3-chloroacrylic acid)                   | Metabolite of 1,3-dichloropropene (compound No. 1-34) | (47)       |
|                            | -COONa       | 4-4          | 2-propenoic acid, 3-chloro-, sodium salt (sodium cis-3-chloroacrylate) | Pesticide (defoliant, dessicant) | (3)        |
| HOOC-CC1=CC1-CHO           | -H           | 4-5          | 2-butenoic acid, 2,3-dichloro-4-oxo- (mucochloric acid)              | (Not found)                   | (2)        |
|                            |              | 4-6          | bis[3,4-dichloro-2(5H)-furanone], 5,- 5'-dioxy- (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)        |
|                            |              | 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)    |
|                            |              | 4-9          | 1,4-naphthalenedione, 2,3-dichloro- (dich lone, 2,3-dichloro-1,4-naphthaquinone) | 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 |
|-----------|-------------|--------------|-------|-------------------------------|------------|
| ![Structure 1](image1) | R | 4-10 | mollisin | Mollisia caesia (fungi); fungicidal activity | (48,49) |
| ![Structure 2](image2) | -- | 4-11 | sclerotiorin | Penicillium sclerotiorum, P. multicolor, P. implicatum (fungi) | (48) |
| ![Structure 3](image3) | -- O-CO-CH₂-CH(CH₃)₂ | 4-12 | isobutyl xanthomonadin I | Xanthomonus sp. (bacteria) | (50) |
| ![Structure 4](image4) | (R₂)₂-P-OR₁ | 4-13 | phosphoric acid, 2-chloro-3(diethylamino)-1-methyl-3-oxo-1-propenyl dimethyl ester (trans-phosphamidon, phosphamidon, 2-chloro-2-diethylcarbamoyl-1-methylvinyl dimethyl phosphate) | Registered pesticide (insecticide) | (1,2,3) |
| ![Structure 5](image5) | C₂H₅O⁻ | 4-14 | phosphoric acid, 3-chloro-4-methyl-2-oxo-2H-1-benzopyran-7-yl diethyl ester (coumaphos-0-analog, 3-chloro-7-hydroxy-4-methylcoumarin diethyl phosphate) | Drug (ophthalmic anti-cholinesterase; veterinary -- anthelmintic) | (2) |
| ![Structure 6](image6) | -- O(C₂H₅)₂ | 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) |
| ![Structure 7](image7) | -- | 4-16 | androst-4-en-3-one, 17-(acetyloxy)-4-chloro-, (1/8) (4-chloroestosterone acetate, clostebol acetate) | Drug (anabolic) | (2) |

(continued)
| Structure | Substituents | Compound No. | Names | Present or past uses; sources | References |
|-----------|-------------|--------------|-------|-------------------------------|------------|
| ![Structure](image) | R R<sub>1</sub> | 4-17 | pregn-4,6-diene-3,20-dione, 17-(acetyl-oxy)-6-chloro- (chlordaninone acetate, 6-chloro-6-dehydro-1α-hydroxy-progesterone acetate) | Drug (progestan; veterinary -- estrus regulator) | (2,7) |
| ![Structure](image) | -H -H | 4-18 | 3'H-cyclopropa[1,2]pregn-1,4,6-triene-3,20-dione, 17-(acetyl-oxy)-6-chloro-1,2-dihydro- (cyproterone acetate, methyleneclormadinone, SH 714) | Drug (antiandrogen) | (2) |
| ![Structure](image) | R R<sub>1</sub> R<sub>2</sub> | 4-19 | 4(1H)-pyridinone, 3,5-diodo- (iopypdone, 3,5-diodopyridine) | Medical diagnostic (radiopaque medium, bronchographic) | (2) |
| ![Structure](image) | -H -H | 4-20 | 4(1H)-pyridinone, 1-(2,3-dihydroxypropyl)-3,5-diodo- (iopypold) | Medical diagnostic (radiopaque medium, bronchographic) | (2) |
| ![Structure](image) | -H -H | 4-21 | 1(4H)-pyridineacetic acid, 3,5-diodo-4-oxo-propyl ester (propyliodone, propiodione) | Medical diagnostic (radiopaque medium) | (1,2,7) |
| ![Structure](image) | -H -H | 4-22 | 1(4H)-pyridineacetic acid, 3,5-diodo-4-oxo- compound with 2,2'-iminodiethanol (1:1) [iodopyracet, diodone, bis(hydroxyethyl)ammonium 3,5-diodo-4-pyridone-N-acetate | Medical diagnostic (radiopaque medium, urographic; veterinary -- same) | (1,2,7) |
| ![Structure](image) | 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-diodo-1-methyl-4-oxo- disodium salt (sodium iodomethamate, iodoxyl) | Medical diagnostic (radiopaque medium) | (2) |
| ![Structure](image) | (CH<sub>3</sub>)<sub>3</sub>-C1 -CH<sub>3</sub> -H | 4-24 | 2,4(1H,3H)-pyrimidinedione, 5-chloro-3-(1,1-dimethyl)6-methyl (terbacil, 3-tert-butyl-5-chloro-6-methyl-uracil) | Registered pesticide (herbicide) | (2,3) |
### Table 4 (cont.)

| Structure | Substituents | Compound No. | Names | Present or past uses; sources | References |
|-----------|--------------|---------------|-------|------------------------------|------------|
| R_1 R_2 R_3 |              | 4-25          | 2,4(1H,3H)-pyrimidinedione, 5-fluoro- (5-fluorouracil, 5-FU, FU) | Drug (antineoplastic agent) | (2,7,8) |
| H^- F^- H^- H^- |            | 4-26          | 2,4(1H,3H)-pyrimidinedione, 5-bromo- (5-bromouracil, 5-BU, BU) | Experimental DNA-incorporatable pyrimidine analog | (51) |
| H^- Br^- H^- H^- |           | 4-27          | uridine, 2'-deoxy-5-fluoro- (flouxuridine, 5-fluorouracil deoxyriboside, 5-FUDR, FUDR) | Drug (antiviral) | (2) |
| H^- I^- H^- |             | 4-28          | uridine, 2'-deoxy-5-ido- (idoxuridine, 5-iodouracil deoxyriboside, IDU, IUDR) | Drug (ophthalmic anti-viral) | (2) |

### Table 5. Related halogenated compounds

| Structure | Substituents | Compound No. | Names | Present or past uses; sources | References |
|-----------|--------------|---------------|-------|------------------------------|------------|
| Epoxides  | R R_1 R_2 R_3 | 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^- 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^- | -Cl           | 5-3 oxirane, 1,2-dichloro-, cis- (cis-1,2-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 R1 R2 R3 |             | 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) | (52,55,37) |
| -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, perfluoroethene oxide, TPEO) | Synthesis of dimers to polymers (Freon E -- coolants for electronic devices) | (1) |
| -F -F -F -CF3 | 5-8 oxirane, trifluoro(trifluoromethyl)- (hexafluoropropylene oxide, perfluoropropylene oxide, HFPO) | Polymer synthesis (lubricating oils and greases) | (1) |
| -- | -- | 5-9 pacifenol | Laurencia pacifica, L. johnstonii, Aplysia californica | (58,59) |
| -- | -- | 5-10 johnstonol | L. pacifica, L. johnstonii, A. californica | (58,60) |
| -- | -- | 5-11 prepacifenol epoxide | L. pacifica, L. johnstonii, A. californica | (43,58) |

(continued)
| Structure | Substituents | Compound No. | Names | Present or past uses; sources | References |
|-----------|-------------|--------------|-------|------------------------------|------------|
| ![Structure](image1) | --          | 5-12         | johnstandiol               | A. californica | (58) |
| ![Structure](image2) | --          | 5-13         | pacifidiene            | A. californica (in vivo dehydration of pacifenol within the digestive gland) | (61) |
| ![Structure](image3) | --          | 5-14         |                   | A. californica (secondary product from pacifenol, via pacifidiene, within the digestive gland) | (61) |
| ![Structure](image4) | CH₂Cl-CHO   | 5-15         | acetaldehyde, chloro- (2-chloroacet-aldehyde) | 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) |
| ![Structure](image5) | CH₂Cl₂-CHO  | 5-16         | acetaldehyde, dichloro- | Synthesis of insecticides; proposed product of rearrangement of both cis- and trans-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 |
|-----------|-------------|-------------|-------|-------------------------------|------------|
| X         |             | 5-17        | acetaldehyde, trichloro- (chiral) | Synthesis of chloral hydrate and DDT; [chiral hydrate is a drug (sedative)]; proposed in vivo product of rearrangement of trichloroethylene epoxide; rearrangement product via Lewis acids (1,2,7,8,52) |            |
| CCl₃-CHO  | --          | 5-17        | acetaldehyde, trichloro- (chiral) | Synthesis of chloral hydrate and DDT; [chiral hydrate is a drug (sedative)]; proposed in vivo product of rearrangement of trichloroethylene epoxide; rearrangement product via Lewis acids (1,2,7,8,52) |            |
| CH₂X-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) |            |
| -Br       | 5-19        | ethanol, 2-bromo- (ethylene bromohydrin) | Synthesis (1,2) |            |
| Alkynes   |             |             |       |                               |            |
| CX≡CX     | -Br         | 5-20        | ethyne, 1,2-dibromo- (dibromoacetylene, dibromoethylene) | Synthesis (1) |            |
| -I        | 5-21        | ethyne, 1,2-diiodo- (diiodoacetylene) | Synthesis; poison vapor (1) |            |
| CH₃-CH₂-C-CHBr | --     | 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)- (haloprogyn, 2,4,5-trichlorophenyl 1-iodopropargyl ether) | Drug (antibacterial) (2,7,8) |            |
| C-Cl      | --          | 5-24        | 19-norpregna-4,9-dien-20-yn-3-one, 21-chloro-17-hydroxy-, (17A) (ethyneronone, MK 665) | Drug (progestin) (2) |            |
| CH₃OH     |             |             |       |                               |            |
| Structure | Substituents | Compound No. | Names | Present or past uses; sources | References |
|-----------|-------------|--------------|-------|-------------------------------|------------|
| **Allylic compounds** | | | | | |
| | | 5-25 | 1-propene, 3-chloro- (allyl chloride, 1-chloro-2-propene, 2-propenyl chloride, chloroallylene) | Polymer and other synthesis | (1,2) |
| | | 5-26 | 1-propene, 3-bromo- (allyl bromide) | Polymer and other synthesis | (1,2) |
| | | 5-27 | silane, trichloroethenyl- (vinyl trichlorosilane, vinylsilicon trichloride, VICS) | Synthesis of silicon adhesives | (1) |
| | | 5-28 | 1-propene, 3-chloro-2-methyl- (3-methylallyl chloride, 3-chloroisobutylene, MAC) | Polymer and other synthesis; pesticide (fungit) | (1,2) |
| | | 5-29 | benzeneethanamine, α-methyl-N-(2,2,2-trichloroethylidene) [amphecloral, α-methyl-N-(2,2,2-trichloroethylidene)-phenylethlamide] | Drug (anorexic) | (2) |
| **Allylic alkynes** | | | | | |
| | X | 5-30 | 1-propyne, 3-chloro- (propargyl chloride) | Synthesis | (1,2) |
| | | 5-31 | 1-propyne, 3-bromo- (propargyl bromide) | Synthesis; registered pesticide (soil fungit) | (1,3) |
| | | 5-32 | carboxylic acid, (3-chlorophenyl)-4-chloro-2-butynyl ester (barban, barbamate, 4-chloro-2-butynyl-3-chlorocarb-banilate) | Registered pesticide (herbicde and plant growth regulator) | (2) |
| Structure | Substituents | Compound No. | Names | Present or past uses; sources | References |
|-----------|-------------|--------------|-------|-------------------------------|------------|
| R         | R<sub>1</sub> | 6-1 oxirane, (ethylene oxide, 1,2-epoxy-ethane, dimethylene oxide, ETO) | Synthesis; registered pesticide (fumigant, insecticide, fungicide); petroleum demulsifier; equipment sterilization; rocket propellant | (1,2,3) |
| -H        | -H          | 6-2 oxirane, methyl- (propylene oxide, 1,2-epoxypropane) | Polymer and other synthesis; registered pesticide (fumigant, insecticide, soil sterilant); solvent | (1,2,3) |
| -H        | -CH<sub>3</sub> | 6-3 oxirane, chloromethyl- (epichlorhydrin, α-epichlorhydrin, 1-chloro-2,3-epoxypropane, γ-chloropropylene oxide, (chloromethyl)ethylene oxide, epi) | Polymer and other synthesis; registered pesticide (fumigant, insecticide); solvent; curing agent for propylene based rubbers; antioxidant in some trichloroethylene preparations | (1,2,3, 63) |
| -H        | -CH<sub>2</sub>CH<sub>3</sub> | 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) |
| -H        | -CH<sub>2</sub>OH | 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) |
| -H        | -CH-CH<sub>2</sub> | 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) |
| Structure   | Substituents | Compound No. | Names                                                                 | Present or past uses; sources | References |
|-------------|--------------|--------------|----------------------------------------------------------------------|-------------------------------|------------|
| R           | R_1          | 6-8          | 7-oxabicyclo(4.1.0)heptane, 3-oxiranylid- (vinylcyclohexene dioxide, vinylcyclohexane dioxide) | Polymer and other synthesis | (1)        |
| -H          | -H           | 6-9          | oxirane, 1,2-dimethyl- (2,3-butylene oxide, 2,3-epoxybutane)           | Synthesis                     | (1)        |
| -CH_3       | -CH_3        | 6-10         | aziridine (ethyleneimine, azacyclopropane, dimethyleneimine, EI)       | Polymer and other synthesis   | (1,2)      |
| -H          | -H           | 6-11         | aziridine, 2-methyl- (propyleneimine, 2-methylethyleneimine)           | Synthesis                     | (1)        |
| -H          | -CH_3        | 6-12         | aziridine, 2-ethyl- (2-ethylenimine)                                  | Synthesis                     | (1)        |
| -CH_2CH_2OH | -H           | 6-13         | l-aziridineethanol [N-(2-hydroxyethyl)ethyleneimine]                    | Synthesis                     | (1)        |
| -CH_2CH=CH=CH_2 | -H      | 6-14         | l-aziridineethanol, o-ethyl- (o- vinyl-1-aziridineethanol, 1-ethyleneimino-2-hydroxy-3-butene) | Experimental neoplastic drug  | (2)        |

Nonconjugated and conjugated alkenes

| Structure | Substituents | Compound No. | Names                                                                 | Present or past uses; sources | References |
|-----------|--------------|--------------|----------------------------------------------------------------------|-------------------------------|------------|
| CH_2=CHR_1 | -H           | 6-15         | ethene (ethylene, elayl, bicarburetted hydrogen, olefiinant gas)      | Polymer and other synthesis; drug (veterinary and human anesthetic); welding and cutting metals; refrigerant; acceleration of fruit ripening | (1,2,3)    |
| -H        | -OCH_3       | 6-16         | ethene, methoxy- (methyl vinyl ether, MVE)                            | Polymer synthesis; plasticizer | (1)        |
| -H        | -O-CH_2=CH_2 | 6-17         | ethene, 1,1'-oxybis- (vinyl ether, divinyl ether, divinyl oxide)       | Polymer synthesis; drug (anesthetic - vincombinum, 75% ethyl ether + 22% vinyl ether) | (1,2,4)    |
| -H        | -O-C-CH_3    | 6-18         | acetic acid, ethenyl ester (vinyl acetate, vinyl A monomer, 1-acetoxyethylene, VyAc) | Polymer synthesis             | (1,2)      |
| Structure | Substituents | Compound No. | Names | Present or past uses; sources | References |
|-----------|-------------|--------------|-------|-------------------------------|------------|
| CH₂=CHR₁ | -H          | 6-19         | 1-propene (propylene, methylethylene) | Polymer and other synthesis; polymer gasoline | (1,2)      |
|           | -CH₃        |              |       |                               |            |
|           | -CHO        | 6-20         | 2-propanal (acrolein, acrylaldehyde, acraldehyde, allyl aldehyde) | Polymer and other synthesis; registered pesticide (herbicide, fungicide); tear gas; warning agent in methyl chloride refrigerant | (1,2,3)   |
|           | -COOH       | 6-21         | 2-propenoic acid, (acrylic acid, acroleic acid, vinyl formic acid) | Polymer synthesis | (1,2) |
|           | -CONH₂      | 6-22         | 2-propenamide (acrylamide) | Polymer and other synthesis; flocculent; sewage and waste treatment; permanent press fabrics | (1,2) |
|           | -CN         | 6-23         | 2-propenenitrile (acrylonitrile, vinyl cyanide, cyanoethylene) | Polymer and other synthesis; modifier of natural fiber; registered pesticide (fungigant, insecticide) | (1,2,3) |
|           | -CH₂-CH₃    | 6-24         | 1-butene (α-butylene, ethylethylene) | Polymer and other synthesis | (1,2) |
|           | -CH=CH₂     | 6-25         | 1,3-butadiene (vinylethylene, bivinyl, ethene) | Polymer and other synthesis | (1,2) |
|           | -C-CH₃      | 6-26         | 3-butene-2-one (methyl vinyl ketone, methylene acetone) | Polymer and other synthesis | (1,2) |
|           |             | 6-27         | benzene, ethenyl- (styrene, phenylethylene, vinyl benzene, styrol, cinnamime) | Polymer and other synthesis | (1,2) |
|           |             | 6-28         | cyclohexene, 4-ethenyl- (4-vinylcyclohexene, 1-vinyl-3-cyclohexene) | Polymer and other synthesis; a butadiene dimer | (1)       |

(continued)
| Structure   | Substituents | Compound No. | Names                                                                 | Present or past uses; sources                      | References |
|------------|-------------|--------------|----------------------------------------------------------------------|---------------------------------------------------|------------|
| CH₂=CHR₁   | -H          | 6-29         | 7-oxabicyclo(4.1.0)heptane, 3-ethenyl- (vinylcyclohexene monoxide, vinylcyclohexane monoxide) | Polymer and other synthesis                        | (1)        |
| -CH₃       | -CH₃        | 6-30         | 1-propene, 2-methyl- (isobutene)                                      | Polymer and other synthesis                        | (1)        |
| -CH₃       | -CH₂-CH₃    | 6-31         | 1-butene, 2-methyl-                                                  | Synthesis                                         | (1)        |
| -CH₃       | -CH=CH₂     | 6-32         | 1,3-butadiene, 2-methyl- (isoprene)                                  | Polymer and other synthesis; "natural" rubber      | (1,2)      |
| -CH₃       | O           | 6-33         | 2-propenoic acid, 2-methyl-, methyl ester (methylmethacrylate, MMA)   | Polymer synthesis; impregnation of concrete        | (1)        |
| -CH₃       | -C=O-CH₃    | 6-34         | 1-buten-3-yn, 2-methyl- (isopropenyl-acetylene)                       | Synthesis; specialty fuel                         | (1)        |
| -CH₃       | -C≡CH       | 6-35         | benzene, 1-(methylethenyl)-(α-methyl-styrene, 2-phenyl-1-propene, α-methyl-styrol) | Polymer synthesis                                 | (1)        |
| -CN        | O           | 6-36         | 2-propenoic acid, 2-cyano- methyl ester (mercurate, methyl-2-cyanoacrylate) | Polymer and adhesive synthesis; surgical aid (tissue adhesive) | (1,2)      |
| -CN        | -CH₂-CH₂-CN | 6-37         | 1,5-pentanedicarbonitrile, 2-methylene- (methyleleneglutaronitrile, 2,4-dicyano-1-butene) | Polymer and other synthesis; acrylonitrile dimer   | (1)        |
| CH₃-CH=CHR₁ | -H          | 6-38         | 2-butene (sym-dimethylethylene, β-butylene, "high-boiling" butene-2) | Synthesis; cross-linking agent; polymer gasoline    | (1,2)      |
| -H         | -CHO        | 6-39         | 2-butenal (crotonaldehyde, trans-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)
| Structure | Substituents | Compound No. | Names | Present or past uses; sources |
|-----------|-------------|--------------|-------|------------------------------|
| \( \text{CH}_3\text{CH}=\text{CH} \text{R}_1 \) | \(-\text{H}\) | \(-\text{COOH}\) | 6-60 | 2-butenoic acid, (crotonic acid, \( \beta \)-methylacrylic acid) Polymer and other synthesis (1,2) |
| \( \text{CH}_3\text{CH}=\text{CH} \text{R}_1 \) | \(-\text{CH}_3\) | \(-\text{CH}_3\) | 6-61 | 2-butene, 2-methyl- (\( \beta \)-amylene, amylene, trimethylene) Synthesis; drug (dental and surgical anesthetic) (1,2) |
| \( \text{CH}_3\text{CH}=\text{CH} \text{R}_1 \) | | | 6-62 | 2-butene-1,4-dione, 1,4-diphenyl- (trans-1,2-dibenzylethylene) Synthesis; bactericide; enzyme inhibitor (1) |
| \( \text{CH}_3\text{CH}=\text{CH} \text{R}_1 \) | | | 6-63 | cyclopentene Polymer and other synthesis (1) |
| \( \text{CH}_3\text{CH}=\text{CH} \text{R}_1 \) | | | 6-64 | 1,3-cyclopentadiene Polymer and other synthesis including organometallics (1,2) |
| \( \text{CH}_3\text{CH}=\text{CH} \text{R}_1 \) | | | 6-65 | cyclohexene Synthesis; catalyst solvent; extraction of oils; suggested stabilizer for high octane gasoline (1,2) |
| \( \text{CH}_3\text{CH}=\text{CH} \text{R}_1 \) | | | 6-66 | 1H-imidazole-3-ethanol, 2-methyl-5-nitro- [metronidazole, 1-(2-hydroxyethyl)-2-methyl-5-nitroimidazole] Drug [antiprotozoal (trichomonas); veterinary -- antiprotozoal, treponemal] (2,7,8) |
| \( \text{CH}_3\text{CH}=\text{CH} \text{R}_1 \) | \(-\text{H}\) | \(-\text{CN}\) | 6-67 | 2-propynitrile (cyanoacetylene) Synthesis (64,65) |
| \( \text{CH}_3\text{CH}=\text{CH} \text{R}_1 \) | \(-\text{H}\) | \(-\text{CH}_3\) | 6-68 | 2-propyne [methylacetylene (stabilized with propadiene)] Industrial fuel gas for cutting, welding, brazing, heat treating and metallizing (1) |
| \( \text{CH}_3\text{CH}=\text{CH} \text{R}_1 \) | \(-\text{H}\) | \(-\text{CH}_2\text{OH}\) | 6-69 | 2-propyn-1-ol (propargyl alcohol) Synthesis; pesticide (soil fumigant, insecticide); corrosion inhibitor; solvent stabilization (1,2,3) (continued) |
| Structure | Substituents | Compound No. | Names | Present or past uses; sources | References |
|-----------|-------------|--------------|-------|-----------------------------|------------|
| R         | R'          |              |       |                             |            |
| CR-<CR1   | -H          | HO           | 6-50  | cyclohexanol, 1-ethynyl- (1-ethynyl-1-cyclohexanol) | Ilizer; prevents hydrogen embrittlement of steel; laboratory reagent | (1,2) |
| -H        | H2N-C-O     |              | 6-51  | cyclohexanol, 1-ethynyl-, carbamate (ethinamate, 1-ethynylcyclohexyl carbamate) | Synthesis; stabilization of chlorinated organic compounds; corrosion inhibitor for mineral acids | (1,2) |
| -H        | OH          |              | 6-52  | 19-norpregna-1,3,5(10)-trien-20-yn-3,17-diol, (17A) (ethynylestradiol) | Drug (estrogen), veterinary -- (estrogenic hormone therapy) | (1,2) |
and the Pesticide Index (3). Each report 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 uninvited, 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.

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-; α, β ... and 1,2 ...; inverted forms such as bromochloro- and chlorobromo-; abbreviated names as in dibromodioethene (which is ambiguous) and 1,2-dibromo-1,2-diodoethene, 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 triphenylethlenes [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 alkenes [3].

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

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

REFERENCES

1. Hawley, G. G., Ed. The Condensed Chemical Dictionary, 9th ed., Van Nostrand Reinhold Co., New York, 1977.
2. Windholz, M., et al., Eds. The Merck Index: An Encyclopedia of Chemicals and Drugs, 9th ed. Merck & Co., Rahway, N. J., 1976.
3. Wiswesser, W. J., Ed. Pesticide Index, 5th ed. Entomological Society of America, College Park, Md., 1976.
4. Marler, E. E. J. Pharmacological and Chemical Synonyms, 6th ed. Excerpta Medica, Amsterdam, 1976.
5. Christensen, H. E. Registry of Toxic Effects of Chemical Substances. National Institute for Occupational Safety and Health, Rockville, Md., 1976.
6. Abstracts on Health Effects of Environmental Pollutants. Chemical Index Guide, BIOSIS, Biological Abstracts, Philadelphia, 1975.
7. APhA Drug Names, American Pharmaceutical Association, Washington, D. C. 1976.
8. Physicians’ Desk Reference, 31st ed. Medical Economics Co., Oradell, N. J., 1977.
9. Hamilton, A., and Hard, H. L. Industrial Toxicology, 3rd ed. Publishing Sciences Group, Inc., Acton, Mass., 1974.
10. Dictionary of Organic Compounds, 4th ed. Oxford University Press, New York, 1965.
11. Chem. Abstracts Service Collective Indexes, American Chemical Society, Washington, D. C.
12. Freundt, K. J., Liebaldt, G. P., and Lieberwirth, E. Toxicity studies on trans-1,2-dichloroethylene. Toxicology 7: 141 (1977).
13. Levek, R. P., and Williams, D. O. Flame retardants. In: Modern Plastics Encyclopedia, Vol. 52, No. 10A, 200, 1975.
14. Van Dyke, R. A. Dechlorination mechanisms of chlorinated olefins. Environ. Health Perspect. 21: 121 (1978).
15. Mellin, I. Industrial Solvents Handbook, 2nd ed. Noyes Data Corp., Park Ridge, N. J., 1977.
16. Castro, C. E., and Belser, N. O. Hydrolysis of cis- and trans-1,3-dichloropropene in wet soil. J. Agr. Food Chem. 14: 69 (1966).
17. Farm Chemicals Handbook. 1975. Meister Publishing Co., Willoughby, Ohio, 1975.
18. Johnson, O. Pesticides, 72. Chemical Week (June 21, 1972).
19. Jensen, S., et al. Chlorinated by-products from vinyl chloride production: a new source of marine pollution. F.A.O. Technical Conference on Marine Pollution and Its Effects on Living Resources and Fishing, Rome, Dec., 1970: F1R:MP/70/E88, 8 pp.
20. Clary, J. J. Toxicology of chloropropane, 1,3-dichlorobutene-2, and 1,4-dichlorobutene-2. Environ. Health Perspect. 21: 261 (1978).
21. Clayton, J. W., Jr., Toxicology of the fluorooalkanes: review and research needs. Environ. Health Perspect. 21: 247 (1978).
22. United States Environmental Protection Agency. Hexachlorobenzene and hexachlorobutadiene pollution from chlorocarbon processing. Survey of Industrial Processing Data, Task I; Final Report, EPA-56013-75-003, June, 1975.
23. Elliott, M., et al. Potent pyrethroid insecticides from modified cyclopropane acids. Nature 244: 456 (1973).
24. Elliott, M. Properties and applications of pyrethroids. Environ. Health Perspect. 14: 3 (1976).
25. Ruzo, L. O., and Casida, J. E. Metabolism and toxicology of pyrethroids with dihalovinyl substituents. Environ. Health Perspect. 21: 277 (1978).
26. Brown, D. G., Bodenstein, O. F., and Norton, S. J. New potent pyrethroid: bromethrin. J. Agr. Food Chem. 21: 767 (1973).
27. Brown, D. G., Bodenstein, O. F., and Norton, S. J. Halopyrethroids: II. A difluoropyrethroid. J. Agr. Food Chem. 23: 115 (1975).
28. Elliott, M., et al. A photostable pyrethroid. Nature 246: 169 (1973).
29. Elliott, M., et al. Radiosynthesis and metabolism in rats of the 1R isomers of the insecticide permethrin. J. Agr. Food Chem. 24: 270 (1976).
30. Elliott, M., et al. Synthetic insecticide with a new order of activity. Nature 248: 710 (1974).
31. Barnes, J. M., and Verschoyle, R. D. Toxicity of new pyrethroid insecticide. Nature 248: 711 (1974).
32. Owens, J. D. Absolute configuration of the potent insecticide α-cyano-3-phenoxybenzyl cis-2,2-dimethyl-3-(2,2-dibromovinyl)cyclopropene carboxylate by X-ray crystal structure analysis. J. Chem. Soc. Chem. Commun. 1974: 859.
33. Goodman, L. S., and Gilman, A., Eds., The Pharmacological Basis of Therapeutics, 5th ed. The Macmillan Co., London, 1975.
34. Friedman, L., and Shibko, S. I. Adventitious toxic factors in processed food. In: Toxic Constituents of Plant Foods, I. E. Liener, Ed., Academic Press, New York, 1969, p. 349.
35. McKinney, L. L., Edridge, A. C., and Cowan, J. C. Cysteinethioethers from chloroethylenes. J. Amer. Chem. Soc. 81: 1423 (1959).
36. Strafuss, A. C., and Sautter, J. H. Clinical and general pathological findings of aplastic anemia associated with 5-(dichlorovinyl-1-cysteine) in calves. Vet.Res. 28: 25 (1967).
37. Rando, R. R. 3-Bromoallylalnine induced irreversible inhibition of monamine oxidase. J. Amer. Chem. Soc. 95: 4438 (1973).
38. Campbell, W. C., and Mrozik, H. Antiparasitic agents. Ann. Repts. Med. Chem. 9: 115 (1974).
39. Usdin, E. D., Efron, D. H. Psychotropic Drugs and Related Compounds, 2nd ed. DHEW Publ. No. (HSM) 72-9074, 1972.
40. Francis, J. E. Antihypertensive agents. Ann. Repts. Med. Chem. 9: 57 (1974).
41. Bloch, A. Antineoplastic agents. Ann. Repts. Med. Chem. 9: 139 (1974).
42. Street, J. C., and Blau, S. E. Oxychlorodane: accumulation in rat adipose tissue on feeding chlorode isomers or technical chlorodane. J. Agr. Food Chem. 20: 305 (1972).
43. Fenical, W. Halogenation in the Rhodophyta: a review. J. Phycol. 11: 245 (1975).
44. Stallard, M. O., and Faulkner, D. J. Chemical constituents of the digestive gland of the sea hare Aplysia californica. I. Importance of diet. Comp. Biochem. Physiol. 49B: 25 (1974).
45. González, A. G., et al. Evidence for the biogenesis of halogenated chamigrenes from the red alga Laurencia ob- stusa. Tetrahedron Letters No. 35: 3051 (1976).
46. McConnell, O., and Fenical, W. Halogen chemistry of the red alga Asparagopsis. Phytochemistry 16: 367 (1977).
47. Belser, N. O., and Castro, C. E. Biodehalogenation—the
metabolism of the nematocides cis- and trans-chloroallyl alcohol by a bacterium isolated from soil. J. Agr. Food Chem. 19: 23 (1971).

48. Miller, M. W. The Pfizer Handbook of Microbial Metabolites. McGraw-Hill, New York, 1961, p. 249.

49. van der Kerk, G. J. M., and Overeem, J. C. M. Mollisin, a dichloronaphthoquinone derivative produced by the fungus Mollisia caesia. Rec. Trav. Chim. 76: 425 (1957).

50. Andrewes, A. G., et al. Structure of xanthomonadin 1, a novel dibrominated aryl-polyene pigment by the bacterium Xanthomonas juglandis. Tetrahedron Letters 45: 4023 (1976).

51. Goldstein, A., Aronow, L., and Kalman, S. M. Principles of Drug Action: The Basis of Pharmacology, 2nd ed. John Wiley and Sons, New York, 1974, p. 117.

52. Bonse, G., and Henschler, D. Chemical reactivity, biotransformation and toxicity of polychlorinated aliphatic compounds. Crit. Rev. Toxicol. 4: 395 (1976).

53. Elmore, J. D., et al. Vinyl chloride mutagenicity via the metabolites chloroacrolein and chloroacetaldehyde monomer hydrate. Biochim. Biophys. Acta 442: 405 (1976).

54. Bolt, H. M., et al. Pharmacokinetics of vinyl chloride in the rat. Toxicology 7: 179 (1977).

55. Leibman, K. C., and Ortiz, E. Metabolism of halogenated ethylenes. Environ. Health Perspect. 21: 91 (1978).

56. Hathway, D. E. Comparative mammalian metabolism of vinyl and vinylidine chlorides in relation to oncogenic potential. Environ. Health Perspect. 21: 55 (1978).

57. Van Duuren, B. L. Chemical structure, reactivity, and carcinogenicity of halohydrocarbons. Environ. Health Perspect. 21: 17 (1978).

58. Faulkner, D. J., Stallard, M. O., and Ireland, C. Pre-pacifenol epoxide, a halogenated sesquiterpene diepoxide. Tetrahedron Letters No. 40: 3571 (1974).

59. Sims, J. J., et al. Marine natural products. I. Pacifenol, a rare sesquiterpene containing bromine and chlorine from the red alga, Laurencia pacifica. J. Amer. Chem. Soc. 93: 3774 (1971).

60. Sims, J. J., et al. Marine natural products III. Johnstonol, an unusual halogenated epoxide from the red alga Laurencia johnstonii. Tetrahedron Letters No. 3: 195 (1972).

61. Stallard, M. O., and Faulkner, D. J. Chemical constituents of the digestive gland of the sea hare Aplysia californica. II. Chemical transformations. Comp. Biochem. Physiol. 49B: 37 (1974).

62. Rosenkranz, H. S. The mutagenicity of olefins and their derivatives. Environ. Health Perspect. 21: 79 (1978).

63. Henschler, D., et al. Carcinogenicity of trichloroethylene: fact or artifact? Arch. Toxicol. 37: 233 (1977).

64. Ferris, J. P., Sanchez, R. A., and Orgel, L. E. Studies in prebiotic synthesis. III. Synthesis of pyrimidines from cyanacetylene and cyanate. J. Mol. Biol. 33: 693 (1968).

65. Durrell, W. S., and Bateman, J. H. Heartcut. Chemtech, 7: 495 (Aug. 1977).

326 Environmental Health Perspectives