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ORGANICS IN DRINKING WATER.

PART I.-

LISTING OF IDENTIFIED CHEMICALS

Gregor A. Junk and Sherri E. Stanley

AMES LABORATORY, USERDA
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Date Transmitted: July 1975

PREPARED FOR THE U. S. ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION
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ABSTRACT

This report contains some brief introductory comments concerning organics in drinking water and in other waters which might be used as raw water sources of public drinking waters. The main body of the report is an alphabetical tabulation of 423 organic chemicals which have been reported to be present in various waters. Of this total, 394 are specifically identified and 325 are reported to be present in drinking water. Molecular weights, empirical formulas, structural information and literature citations are included in the tabulation.

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Organics in Drinking Water. Part I.-
Listing of Identified Chemicals

Gregor A. Junk and Sherri E. Stanley

A convenient tabulation of the organic chemicals which have been identified in drinking waters and in other water which might be used as raw water sources of public drinking waters is of interest to toxicologists, analytical chemists, water researchers, water purveyors, regulatory agencies and the general populace. Recently available tabulations have problems in one or more of the following areas: 1) nomenclature; 2) chemical structure; 3) duplications; 4) incompleteness; 5) lack of literature citations; 6) updating. To resolve these problems, all available reports of organics in water were reviewed and the data in these reports were organized, proofed, tabulated and formatted. The results of these efforts evolved into Table I of this report.

The nomenclature problem is largely obviated by the alphabetical listing of trivial, trade and generic names with cross-indexing. The pertinent data are included after the most commonly employed name.

Difficulty in chemical structure is resolved by including empirical and line formulae. Where possible confusion might exist the exact chemical structure is referred to and reproduced in Appendix I.

Duplications have been eliminated by communication with the authors of the original reports when necessary. In some instances only partial chemical characterization is available and this causes some probable overlap. For example one report may have listed a C₃-alkylbenzene while another report listed both iso- and n-propylbenzene. In these cases, the undesignated C₃-alkylbenzene is retained as a separate entry. In general, this situation exists only for the alkylbenzenes, alkyl naphthalenes and alkanes.

The current tabulation is considered complete based on an extensive search of the original U.S.A. literature on drinking water and cross-checks against other tabulations available to the author as of May 1, 1975. No attempt was made to extensively survey either the foreign literature or those reports dealing specifically with waste waters.

The list of references after each entry in Table I can be used to trace the data back to the original reports. However the citation list should not be used to judge the probable distribution of the listed organic chemical. In many cases, two or three citations associated with an entry refer to other compilations all of which used the same original source

reference. In other cases, only a single citation is listed but the organic chemical was detected in several different water supplies.

Additions to the alphabetical listing of organics found in water are usually cumbersome and costly. To resolve this problem, the spacing between letter entries in Table I has been adjusted to include room for a reasonable number of additional entries. This approach conserves space and still retains the gross a,b,c system although any additions will be out of strict alphabetical order.

The present compilation attests to the considerable progress made over the past five years in establishing the profile of organics present in drinking water. As of 1970 a comprehensive listing of organics present in fresh water (85) contained only 35 chemicals. As of May, 1975 the number of identified chemicals in drinking water alone has exploded to over 300. Although this represents significant progress, the list is still not complete and the number of entries will undoubtedly increase in future years. This will occur due more to improved methodology and increased research activity rather than increased levels of pollution. The improved methodologies will include methods for measuring those organic components which currently are excluded by the almost universal choice of gas chromatography for separating the mixture isolated from the water under test. The gas chromatographic procedures generally employed are not capable of detecting thermally labile, highly polar or very high molecular weight constituents. Thus, these components will be added to the tabulation only after the evolution and more extensive use of other separation schemes coupled with improved isolation and detection procedures.

Some data currently available reflect the still incomplete status of the present tabulation. Most drinking waters contain about 5 mg per liter of dissolved organic matter. The total amount of individual organic chemicals detected by gas chromatographic procedures is usually less than 0.5 mg per liter. Thus 90% of the total amount of organic material present in the water is usually not identified.

While this percentage is suggestive of the unknowns still to be resolved in water research, the situation should not be the cause of undue alarm for several reasons. Firstly, many of the toxic and bioaccumulative components in water are expected to be gas chromatographable and the application of current analytical techniques allows for the identification of over 80% by weight of these chromatographable components. Secondly, the low 10% identified is based on total weight and therefore it is not exactly related to the ratio of the number of identified to unidentified components. Thirdly, existing evidence suggests that most of the 90% unidentified materials

are probable soluble humic substances. These might provide beneficial effects which far outweigh any possible health hazard.

Comment

Although Table I is generally devoid of the six shortcomings discussed in the introduction, much helpful information is still missing. Foremost is the absence of amount, distribution, persistence, source and control data. These data are not available from the original literature because the productive past research has stressed the establishment of the profile of organics in water. Minimal efforts have been devoted to the other essential studies. A recent report from the Office of Toxic Substances (81) includes persistence, source and control data for many organics found in water and this effort is expected to continue and expand.

With regard to amounts and distribution much more data are needed. The Environmental Protection Agency (EPA) New Orleans reports (42,92) of amounts and the EPA Reconnaissance Survey (66) of 80 cities for amounts and distributions of volatile C_1 and C_2 halocarbons are the only two extensive reports available.

At present, any attempt to establish distribution from existing reports would end in failure. The results would reflect scientific activity, sample site bias, instrument sensitivity and technological evolution rather than true distribution. The situation with amounts is similar because the only compounds with a valid data base are the C_1 and C_2 haloforms. Based on the EPA study (66) of 80 cities, the distribution and range of amounts are: 100% (0.2-311 $\mu\text{g/l}$) for chloroform; 95% (0.3-116 $\mu\text{g/l}$) for bromodichloromethane; 89% (0.4-100 $\mu\text{g/l}$) for dibromochloromethane; 30% (0.8-92 $\mu\text{g/l}$) for bromoform; 33% (0.2-6 $\mu\text{g/l}$) for 1,2-dichloroethane; and 12% (2-3 $\mu\text{g/l}$) for carbon tetrachloride. For all other chemicals, the amounts are usually not available from the original reports. When available, the sampling frequency is inadequate to establish the validity of the reported amounts. Additionally, the results do not include drinking water supplies which have different raw water sources such as deep wells, shallow wells, flowing rivers, infiltration galleries, lakes and impounded reservoirs.

In spite of these limitations, the available data on amounts can be used to conclude that the identified organic contaminants in drinking water are generally present at less than 10 $\mu\text{g/l}$ (10 ppB). The only exceptions to this estimate are the C_1 and C_2 halocarbons, whose concentrations at times

exceed 300 $\mu\text{g}/\text{l}$, and a few isolated cases of industrial discharges immediately upstream from a surface source of raw water. A further conclusion is that most all identified organic chemicals with boiling points above 150°C are present in drinking water at concentrations below one $\mu\text{g}/\text{l}$.

Summary of Table I

Identified organic chemicals	394
Undesignated organic chemicals	<u>29</u>
Total number of entries	423
Organic chemicals in drinking water	325
In water sources other than drinking water	<u>92</u>
Total number of entries	405

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Table I. LISTING OF ORGANICS FOUND IN DRINKING (TREATED) WATER

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
acenaphthene	$C_{12}H_{10}$ see A1	154	treated well	10
acenaphthylene	$C_{12}H_8$ see A2	152	treated well	10,76
acetaldehyde	C_2H_4O CH_3CHO	44	treated river treated well	42,66,94 66
acetic acid	C_2H_4O CH_3COOH	60	treated river	53 40
acetic anhydride	$C_4H_6O_3$ $(CH_3CO)_2O$	102	treated	77
acetone	C_3H_6O H_3CCOCH_3	58	treated river river treated bottled	42,66,94 2 59,66,68,69,71, 73,75,77,83,84 94
acetophenone	C_8H_8O $C_6H_5(COCH_3)$	120	river treated	48 59,73
acetoveratrone	(see 3,4-dimethoxyacetophenone)			
acetylenebromide	C_2HBr $HC\equiv CBr$	104	treated well	66
acetylenechloride	C_2HCl $HC\equiv CCl$	60	treated well treated river	66 66

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
acetylenedichloride	$C_2H_2Cl_2$ $HCCl=CHCl$	96	treated treated river	2,59,67,73,84 66
*acrylonitrile	C_3H_3N $H_2C=CHC\equiv N$	53	river	37
alachlor	$C_{14}H_{20}O_2NCl$ see A3	269	treated river rivers	92 27
alachlor (2-Cl homologue)	$C_{14}H_{19}O_2NCl_2$ see A4	303	treated	92
alcohols	ROH ROH	unk	treated well tube river	11 28 37
*aldehydes	RCHO RCHO	unk	river	37
aldrin	$C_{12}H_8Cl_6$ see A5	362	river treated	3,38,52,85 52,85
C_9 alkane	C_9H_{20} C_9H_{20}	128	treated	82
* C_{10} alkane	$C_{10}H_{22}$ $C_{10}H_{22}$	142	well	82
C_{11} alkane	$C_{11}H_{24}$ $C_{11}H_{24}$	156	treated	82

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
C ₁₂ alkane	C ₁₂ H ₂₆ C ₁₂ H ₂₆	170	treated	82
*C ₁₃ alkane	C ₁₃ H ₂₈ C ₁₃ H ₂₈	184	well	82
C ₁₄ alkane	C ₁₄ H ₃₀ C ₁₄ H ₃₀	198	treated	82
*C ₁₅ alkane	C ₁₅ H ₃₂ C ₁₅ H ₃₂	212	well	82
C ₁₆ alkane	C ₁₆ H ₃₄ C ₁₆ H ₃₄	226	treated	82
C ₁₇ alkane	C ₁₇ H ₃₆ C ₁₇ H ₃₆	240	treated	82
C ₁₈ alkane	C ₁₈ H ₃₈ C ₁₈ H ₃₈	254	treated	82
C ₁₉ alkane	C ₁₉ H ₄₀ C ₁₉ H ₄₀	268	treated	82
C ₂₀ alkane	C ₂₀ H ₄₂ C ₂₀ H ₄₂	282	treated	82
C ₂₁ alkane	C ₂₁ H ₄₄ C ₂₁ H ₄₄	296	treated	20, 82

COMPOUND NAME	FORMULA STRUCTURE	Mwt.	WATER TYPE	REFERENCES
C ₂₂ alkane	C ₂₂ H ₄₆ C ₂₂ H ₄₆	310	treated	20
C ₂₃ alkane	C ₂₃ H ₄₈ C ₂₃ H ₄₈	324	treated	20, 82
C ₂₄ alkane	C ₂₄ H ₅₀ C ₂₄ H ₅₀	338	treated	20
C ₂₅ alkane	C ₂₅ H ₅₂ C ₂₅ H ₅₂	352	treated	82
C ₂₆ alkane	C ₂₆ H ₅₄ C ₂₆ H ₅₄	366	treated	82
C ₂₇ alkane	C ₂₇ H ₅₆ C ₂₇ H ₅₆	380	treated	82
alkylbenzenes	unk C ₆ H ₅ (R)		treated well treated river	10 42
alkylbenzene- sulfonates	unk (R)C ₆ H ₄ (SO ₃ R)		river treated	47 54
alkylbenzothio- phenc	unk see A6		treated well	10
alkyl-2,3- dihydroindene	unk see A7		treated well	10

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
alkylindan	(see alkyl-2,3-dihydroindene)			
alkylnaphthalenes	unk see A8		treated well	10
* alkylphenols	unk (R)C ₆ H ₄ (OH)		rivers wells	21 21
alkylphthalates	unk see A9		treated well	11
*aniline	C ₆ H ₇ N C ₆ H ₅ (NH ₂)	93	river	29
*anthracene	C ₁₄ H ₁₀ see A10	178	river well	25 82
*C ₁ anthracene	C ₁₅ H ₁₂ see A11	192	river	25
*C ₂ anthracene	C ₁₆ H ₁₄ see A12	206	river	25
atrazine	C ₈ H ₁₄ N ₅ Cl see A13	215	treated treated river	27, 86, 87 42

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
barbital	$C_8H_{12}O_3N_2$ see B1	184	treated	67,71,72,91
behenic acid	$C_{22}H_{44}O_2$ $CH_3(CH_2)_{20}COOH$	340	treated river	55,71
benzaldehyde	C_7H_6O $C_6H_5(CHO)$	106	treated	68,81,91,92
*1,2-benzanthracene	$C_{18}H_{12}$ see B2	228	river	6
benzene	C_6H_6 C_6H_6	78	treated river rain bottled	44,53,59,66,68, 73,79,83,84,94 2, 11 51 94
C_3 -benzene	C_9H_{12} $C_6H_5(C_3H_7)$	120	treated	53
C_5 -benzene	$C_{11}H_{16}$ $C_6H_5(C_5H_{11})$	148	treated	20,53
C_6 -benzene	$C_{12}H_{18}$ $C_6H_5(C_6H_{13})$	162	treated	20
*benzenehexa- chloride	$C_6H_6Cl_6$ see B3	288	river	52,64,71

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
benzenesulfonic acid	$C_6H_6O_3S$ $C_6H_5(SO_3H)$	158	treated river treated	55 67,71,91
*benzidine	$C_{12}H_{12}N_2$ see B4	184	waste	58
benzo[e]pyrene	(see 3,4-benzopyrene)			
*3,4-benzo- fluoranthene	$C_{20}H_{12}$ see B5	252	river	6
*4,5-benzo- fluoranthene	$C_{20}H_{12}$ see B6	252	river	65
*10,11-benzofluor- anthene	$C_{20}H_{12}$ see B7	252	river	6
*11,12-benzofluor- anthene	$C_{20}H_{12}$ see B8	252	river	6,65
benzoic acid	$C_7H_6O_2$ $C_6H_5(COOH)$	122	treated river treated	55 66,91
benzo[j]fluor- anthene	(see 10,11-benzofluoranthene)			
benzo[k]fluor- anthene	(see 11,12-benzofluoranthene)			
1,2-benzo- phenanthrene	(see chrysene)			
benzopyrene isomers	$C_{20}H_{12}$ see B9	252	river treated	1 1, 85

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
1,2-benzopyrene	(see benzopyrene isomers)			
3,4-benzopyrene	$C_{20}H_{12}$ see B10	252	river treated	65 45
benzothiazole	C_7H_5NS see B11	135	rivers treated	2,11 59, 91
benzothiophene	C_8H_6S see B12	134	treated well treated	10 91
*1,12-benzperylene	$C_{22}H_{12}$ see B13	276	rivers	6,65
benzylbutyl- phthalate	(see butylbenzylphthalate)			
BHC	(see benzene hexachloride)			
gamma BHC	(see lindane)			
biphenyl	$C_{12}H_{10}$ see B14	154	river treated lake	24 75 56
bladex	$C_9H_{13}N_6Cl$ see B16	240	treated river	91
borneol	$C_{10}H_{18}O$ see B17	154	river treated	2 73,84
bornyl alcohol	(see borneol)			

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
bromobenzene	C_6H_5Br $C_6H_5(Br)$	156	treated river	59,73,83,84,91 2
bromochlorobenzene	C_6H_4ClBr $(Cl)C_6H_4(Br)$	190	treated river	59,73,83,84,91 2
bromodichloro- methane	$CHCl_2Br$ $HCCl_2Br$	162	treated river treated	16,31,42 53,59,66,67,68, 71,76,79,86,89, 74,94
bromoform	$CHBr_3$ $HCB r_3$	250	bottled treated river treated	31,42 53,66,67,73,76, 79,89,59,74
bromomethane	CH_3Br H_3CBr	94	treated	66,91
2-bromo-2-methyl- propane	(see butylbromide)			
bromophenyl- phenylether	$C_{12}H_9OBr$ see B18	248	treated river	59,73,83,84 2
bromotrichloro- ethylene	C_2Cl_3Br $Cl_2C=CClBr$	208	treated	67
butachlor	$C_{17}H_{26}O_2NCl$ see B19	311	treated	92
butanal	C_4H_8O $H_3C(CH_2)_2CHO$	72	treated	53
1-butanoic acid	(see butyric acid)			

COMPOUND NAME	FORMULA STRUCTURE	Mwt.	WATER TYPE	REFERENCES
butanone	C_4H_8O $CH_3COC_2H_5$	72	treated river treated	42, 53, 66 67, 69
2-butenal	(see crotnaldehyde)			
*t-butylalcohol	$C_4H_{10}O$ $(CH_3)_3COH$	74	well treated river	77 94
butylbenzene	$C_{10}H_{14}$ see B20	134	treated river	59, 73, 83, 84 2
butylbenzene- sulfonamide	$C_{10}H_{15}O_2NS$ see B21	213	treated well	11
*butylbenzoate	$C_{11}H_{14}O_2$ $C_6H_5(COOC_4H_9)$	178	tube river	28 24
butylbenzyl- phthalate	$C_{19}H_{20}O_4$ see B22	312	treated river treated	42 67, 71, 72, 82
t-butylbromide	C_4H_9Br $(CH_3)_3CBr$	136	treated	53
*butylchloroacetate	$C_6H_{11}O_2Cl$ $ClCH_2COOC_4H_9$	150	tube	28
*butylglycollyl- butylphthalate	$C_{18}H_{24}O_6$ see B23	336	tube	28
*2-t-butyl-4- methylphenol	$C_{11}H_{16}O$ see B24	164	rivers wells	21 21

COMPOUND NAME	FORMULA STRUCTURE	Mwt.	WATER TYPE	REFERENCES
butyloctylfumarate	(see octylbutylfumarate)			
butyloctylmaleate	$C_{16}H_{28}O_4$ see B25	284	treated	92
*p-t-butylphenol	$C_{10}H_{14}O$ see B26	150	tube	28
butylphthalyl- butylglycollate	(see butylglycollylbutylphthalate)			
butyraldehyde	(see butanal)			
*butyric acid	$C_4H_8O_2$ $CH_3CH_2CH_2COOH$	88	river	40
C_4 -benzene	$C_{10}H_{14}$ $C_6H_5(C_4H_9)$	134	treated	20,53
camphanol	(see isoborneol)			
α -camphanone	(see camphor)			
camphor	$C_{10}H_{16}O$ see C1	152	treated river	59,73,84 2

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
*caproic acid	$C_6H_{12}O_2$ $CH_3(CH_2)_4COOH$	116	river	40
ε-caprolactam	$C_6H_{11}ON$ see C2	113	treated	59,80
carbon dioxide	CO_2 CO_2	44	treated	79,91
carbon disulfide	CS_2 CS_2	76	treated river treated well	42 66
carbon tetra- chloride	CCl_4 CCl_4	152	treated river	16,42,44,59,66, 67,73,53,79,94 16,42
chloral	C_2HOC_3 Cl_3CCHO	146	treated	70
α-chlordane	$C_{10}H_6Cl_8$ see C3	406	river treated rain	19,38 52,71,92 63
chlordene	$C_{10}H_6Cl_6$ see C4	336	treated	92
2-chloro-4-amino-6- isopropylamino- <u>s</u> - triazine	(see deethylatrazine)			
chlorobenzene	C_6H_5Cl $C_6H_5(Cl)$	112	river treated	2 59,66,73,79 82,83,84,53

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
chlorodibromo- methane	CHClBr_2 HCClBr_2	206	treated river treated bottled	16, 31, 42, 66, 67, 68, 79, 86, 89, 94 59, 76, 71, 74 94
2-chloro-4,6-di- ethylamino-s- triazine	(see simazine)			
2-chloro-2',6'-diethyl- N-(butoxymethyl)- acetanilide	(see butachlor)			
chloroethane	$\text{C}_2\text{H}_5\text{Cl}$ $\text{H}_3\text{CCH}_2\text{Cl}$	64	treated river treated well	66 66
1,2-bis(2-chloro- ethoxy)ethane	(see triglycoldichloride)			
2-chloro-4-ethylamino- 6-isopropyl-s-triazine	(see atrazine)			
2-(4-chloro-6-ethylamino- s-triazin-2ylamino)-2- methylpropionitrile	(see bladex)			
chloroethylether	$\text{C}_4\text{H}_9\text{OCl}$ $\text{ClCH}_2\text{CH}_2\text{OCH}_2\text{CH}_3$	108	treated river	59, 84 2
bis(2-chloroethyl- ether)	$\text{C}_4\text{H}_8\text{OCl}_2$ $(\text{ClCH}_2\text{CH}_2)_2\text{O}$	142	treated treated rivers rivers	42, 73, 76, 78, 84 2, 31, 59 15, 48
2-chloroethyl- methyl ether	$\text{C}_3\text{H}_7\text{OCl}$ $\text{ClCH}_2\text{CH}_2\text{OCH}_3$	94	treated	67, 71
tris(chloroethyl) phosphate	$\text{C}_6\text{H}_{12}\text{O}_4\text{Cl}_3\text{P}$ see C17	284	treated	91

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
chloroform	CHCl_3 HCCl_3	118	treated river rain treated bottled	42, 66, 94 51 16, 44, 53, 59, 66, 67, 68, 71, 73, 74, 75, 76, 79, 83, 86, 88 94
chlorohydroxy- benzophenone	$\text{C}_{13}\text{H}_9\text{O}_2\text{Cl}$ see C5	232	treated river treated	31 59, 76
2-chloro-N- isopropylaceta- nilide	(see propachlor)			
bis(2-chloroiso- propylether)	$\text{C}_6\text{H}_{12}\text{OCl}_2$ see C18	170	rivers treated river treated	15, 48 31, 42 59, 76
chloromethylether	$\text{C}_2\text{H}_5\text{OCl}$ $\text{ClCH}_2\text{OCH}_3$	80	treated	59, 73
chloromethylethyl- ether	$\text{C}_3\text{H}_7\text{OCl}$ $\text{ClCH}_2\text{OCH}_2\text{CH}_3$	94	treated river	59, 84 2
m-chloronitro- benzene	$\text{C}_6\text{H}_4\text{O}_2\text{NCl}$ see C6	157	treated river	59, 73, 84, 92 2
chloropicrin	CO_2NCl_3 Cl_3CNO_2	163	treated	66
chloropropane	$\text{C}_3\text{H}_7\text{Cl}$ $\text{ClCH}_2\text{CH}_2\text{CH}_3$	78	treated	67
1-chloropropene	$\text{C}_3\text{H}_5\text{Cl}$ $\text{ClCH}=\text{CHCH}_3$	76	treated	16

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
3-chloropyridine	C_5H_4NCl see C7	113	treated river	59,73,84 2
$C_{13}H_{22}O$	$C_{13}H_{12}O$ $C_{13}H_{12}O$	184	treated	20
*chrysene	$C_{18}H_{12}$ see C8	228	river	6
1,8-cineole	$C_{10}H_{18}O$ see C9	154	treated	77
o-cresol	C_7H_8O see C10	108	tube treated	28 78
crotonaldehyde	C_4H_6O $H_3CCH=CHCHO$	70	treated	68
cumene	(see isopropylbenzene)			
cyanazine	(see bladex)			
cyanogen chloride	$CNCl$ $ClC\equiv N$	61	treated well treated river treated	66 66 67
cycloheptanone	$C_7H_{12}O$ see C11	112	treated	81
cyclohexane	C_6H_{12} see C12	84	treated	44

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
cyclohexene	C_6H_{10} see C13	82	treated	44
cyclopentadiene	C_5H_6 see C14	66	treated	44
cyclopentane	C_5H_{10} see C16	70	treated	44
cyclopentene	C_5H_8 see C15	68	treated	44
dacthal	$C_{10}H_6Cl_4O_4$ see D47	330	treated	93
*2,4-D	$C_8H_6O_3Cl_2$ see D1	220	river	33
*DDD(TDE)	$C_{14}H_{10}Cl_4$ see D2	318	river lake	33, 38 23
p,p'-DDE	$C_{14}H_8Cl_4$ see D3	316	treated river rain	27, 52, 71, 87, 92 33, 38 63

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
DDT	$C_{14}H_9Cl_5$ see D4	352	river sea lake treated rain	33, 37, 38 22 23 52, 71 63
n-decane	$C_{10}H_{22}$ $CH_3(CH_2)_8CH_3$	142	treated river treated bottled	42 20, 53 94
*decylamine	$C_{10}H_{23}N$ $H_3C(CH_2)_9NH_2$	157	tube	28
deethylatrazine	$C_6H_{10}N_5Cl$ see D8	187	treated	42
DEHP	(see di-2-ethylhexylphthalate)			
dextrose	(see glucose)			
dialkylphthalate	unk see D5		treated	20
*di-n-amylketone	$C_{11}H_{22}O$ $C_5H_{11}COC_5H_{11}$	170	well	77
*diamylphthalate	$C_{18}H_{26}O_4$ see D6	306	tube	28
*1,2,5,6-dibenz- anthracene	$C_{22}H_{14}$ see D7	278	river	17
dibromobenzene	$C_6H_4Br_2$ $C_6H_4(Br)_2$	234	treated river	59, 73, 83, 84 2

COMPOUND NAME	FORMULA STRUCTURE	Mwt.	WATER TYPE	REFERENCES
dibromochloro- methane	(see chlorodibromomethane)			
dibromodichloro- ethane	$C_2H_2Cl_2Br_2$ BrClCHCHClBr	254	treated river	42
*dibutoxyethoxy- ethoxymethane	$C_{13}H_{28}O_4$ see D9	248	rivers	24
2,6-di-t-butyl-p- benzoquinone	$C_{14}H_{20}O_2$ see D52	220	treated river	92
*2,6-di-t-butyl- p-cresol	$C_{15}H_{24}O$ see D48	220	rivers treated tube wells	21 11 28 21
*2,6-di-t-butyl- 4-ethylphenol	$C_{16}H_{26}O$ see D49	234	rivers wells	21 21
*dibutylmaleate	$C_{12}H_{20}O_4$ see D10	228	tube	28
*2,6-di-t-butyl- 4-methoxyphenol	$C_{15}H_{24}O_2$ see D50	236	river wells	21 21
dibutylphthalate	$C_{16}H_{22}O_4$ see D11	278	treated river treated rivers tube lake	42 53,67,71,72, 82 24,25 28 56
1,2-dichlorobenzene	$C_6H_4Cl_2$ see D12	146	treated well treated river	66,82 66

COMPOUND NAME	FORMULA STRUCTURE	Mwt.	WATER TYPE	REFERENCES
1,3-dichlorobenzene	$C_6H_4Cl_2$ see D13	146	river treated river treated well treated	2 42 20, 53, 66 82
1,4-dichlorobenzene	$C_6H_4Cl_2$ see D14	146	treated bottled	42, 66, 73, 82 83, 84 94
2,6-dichloro- benzenecarbonitrile	(see 2,6-dichlorobenzonitrile)			
*2,6-dichlorobenzo- nitrile	$C_7H_3NCl_2$ see D15	171	irriga.	18
dichlorobromo- methane	(see bromodichloromethane)			
1,1-dichloro-2,2- di(p-chlorophenyl) ethylene	(see p,p' DDE)			
dichlorodifluoro- ethane	$C_2H_2Cl_2F_2$ $H_2C_2Cl_2F_2$	134	treated	53,
1,1-dichloroethane	$C_2H_4Cl_2$ H_3CCHCl_2	98	treated treated well	16, 44, 94 66
1,2-dichloroethane	$C_2H_4Cl_2$ $ClCH_2CH_2Cl$	98	treated river treated	42 16, 59, 66, 67, 73, 83
1,1-dichloro- ethylene	$C_2H_2Cl_2$ $Cl_2C=CH_2$	96	treated river treated well	66, 94 66

COMPOUND NAME	FORMULA STRUCTURE	Mwt.	WATER TYPE	REFERENCES
1,2-dichloro- ethylene	(see acetylenedichloride)			
cis-1,2-dichloro- ethylene	$C_2H_2Cl_2$ see D16	96	treated river treated well	66 66
trans-1,2-dichloro- ethylene	$C_2H_2Cl_2$ see D17	96	treated well	66
dichloroethyl ether	(see bis(2-chloroethyl)ether)			
1,1-dichloro-2- hexanone	$C_6H_8OCl_2$ see D18	166	treated	68,81
dichloriodo- methane	$CHCl_2I$ $HCCl_2I$	210	treated	70,74
dichloromethane	CH_2Cl_2 H_2CCl_2	84	treated river treated bottled	42,68,79,94 53,66,71, ,75,77 94
2,4-dichlorophenol	$C_6H_4OCl_2$ see D19	162	treated	68
dichloropropane	$C_3H_6Cl_2$ $C_3H_6Cl_2$	112	treated bottled	16,94 94
1,3-dichloropropane	$C_3H_6Cl_2$ $ClCH_2CH_2CH_2Cl$	112	treated	16
1,3-dichloropropene	$C_3H_4Cl_2$ $ClCH_2CH=CHCl$	110	treated	16,94

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
dicyclopentadiene	$C_{10}H_{12}$ see D20	132	treated	92
dieldrin	$C_{12}H_8OCl$ see D21	378	treated river treated river rain	27, 52, 66, 85, 87 3, 15, 33, 38 42 63
*diethylamine	$C_4H_{11}N$ $(C_2H_5)_2NH$	73	waste (U.S.S.R.)	41
5,5-diethyl- barbituric acid	(see barbital)			
diethylbenzene	$C_{10}H_{14}$ $C_6H_4(C_2H_5)_2$	134	treated well treated	11 68
diethyl ether	$C_4H_{10}O$ $(H_3CCH_2)_2O$	74	treated river treated well bottled	66, 69, 94 66 94
*diethylhexyl- adipate	$C_{22}H_{42}O_4$ see D22	370	river lake	24 56
di-2-ethylhexyl- phthalate	$C_{24}H_{38}O_4$ see D23	390	tube rivers treated river treated lake	28 24, 25 42, 55 67, 71, 72 56
diethylphthalate	$C_{12}H_{14}O_4$ see D24	222	tube treated river well treated	28 42, 55 82 67, 71, 72

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
dihexylphthalate	$C_{20}H_{30}O_4$ see D25	334	treated river treated	42 82
dihydrocarvone	$C_{10}H_{16}O$ see D26	152	treated river	42
2,3-dihydroindene	C_9H_{10} see D27	118	treated well treated	10, 20 76
*diisobutyl carbinol	$C_9H_{20}O$ see D28	144	river treated	48 91
diisobutyl- phthalate	$C_{16}H_{22}O_4$ see D29	278	tube treated river treated	28 42 91
*diisodecyl- phthalate	$C_{28}H_{46}O_4$ see D30	446	river	24
*diisopropyl-p- xylene	$C_{14}H_{22}$ see D31	190	tube	28
dimethoxyaceto- phenone	$C_{10}H_{12}O_3$ see D32	180	treated well	11
*3,4-dimethoxyaceto- phenone	$C_{10}H_{12}O_3$ see D33	180	tube	28
dimethoxybenzene	$C_8H_{10}O_2$ see D34	138	treated	59, 73, 84
dimethoxymethane	$C_3H_8O_2$ $H_2C(OCH_3)_2$	76	treated river	66

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
*dimethylamine	C_2H_7N $(CH_3)_2NH$	45	waste (USSR)	41
dimethylbenzene	C_8H_{10} $C_6H_4(CH_3)_2$	106	treated	31, 42, 53, 68, 76, 79
1,2-dimethylbenzene	C_8H_{10} see D35	106	treated rain bottled	20, 31, 42, 44, 79, 82, 94 51 94
1,3-dimethylbenzene	C_8H_{10} see D36	106	treated rain bottled	20, 31, 42, 44, 79, 82, 94 51 94
1,4-dimethylbenzene	C_8H_{10} see D37	106	treated rain bottled	20, 31, 42, 44, 79, 82, 94 51 94
trans-1,10- dimethyl-9- decalol	(see geosmin)			
dimethyl disulfide	$C_2H_6S_2$ $H_3CS-SCH_3$	94	treated river	66
2,6-dimethyl-4- heptanol	(see diisobutylcarbinol)			
O, O-dimethyl-O- (4-nitro-m-tolyl) phosphorothioate	(see fenitrothion)			
O, O-dimethyl-O(3- methyl-4-nitrophenyl) phosphorothioate	(see fenitrothion)			
1,3-dimethyl naphthalene	$C_{12}H_{12}$ see D38	156	treated	59, 73

COMPOUND NAME	FORMULA STRUCTURE	Mwt.	WATER TYPE	REFERENCES
2,4-dimethylphenol	$C_8H_{10}O$ see D39	122	treated	78
dimethylphthalate	$C_{10}H_{10}O_4$ see D40	194	treated river	42
dimethylsulfoxide	C_2H_6OS $(CH_3)_2S=O$	78	treated	59,73
O-O-dimethyl-O-(2,4,5 trichlorophenyl)phosphorothionate	(see Ronnell)			
4,6-dinitro-2-aminophenol	$C_6H_5O_5N_3$ see D41	199	treated	78
dinitrotoluene	$C_7H_6O_4N_2$ $(CH_3)C_6H_3(NO_2)_2$	182	treated river	59,73,83,84 2
dioctyl adipate	$C_{22}H_{42}O_4$ see D42	370	treated river treated well treated	42 66 68
dioctyl phthalate	$C_{24}H_{38}O_4$ see D43	390	rivers treated	24 82
*1,4-dioxane	$C_4H_8O_2$ see D51	88	well	75,77
diphenylamine	$C_{12}H_{11}N$ see D44	169	treated	27

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
diphenylether	(see phenyl ether)			
diphenylhydrazine	$C_{12}H_{12}N_2$ see D45	184	treated	68
dipropylphthalate	$C_{14}H_{18}O_4$ see D46	250	treated river	42
docosane	$C_{22}H_{46}$ $H_3C(CH_2)_{20}CH_3$	310	treated river treated	55 67,71
docosanoic acid	(see behenic acid)			
n-dodecane	$C_{12}H_{26}$ $H_3C(CH_2)_{10}CH_3$	170	treated river treated	42 20,76
DOP	(see dioctylphthalate)			
dimethyl-2,3,5,6-tetrachloroterephthalate	(see dacthal)			

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
eicosane	$C_{20}H_{42}$ $H_3C(CH_2)_{18}CH_3$	282	treated	20,67,71,72
endo-2-camphanol	(see borneol)			
endo-endo isomer of aldrin	(see isodrin)			
*endosulfan	$C_9H_6O_3Cl_6S$ see E1	404	river	38
endotoxins	polymeric unknown		treated	14
endrin	$C_{12}H_8OCl_6$ see E2	378	treated river rivers treated	42 3,9,38 52,71
*esters	unk $RCOOR$		river	37
ethanol	C_2H_6O H_3CCH_2OH	46	treated river treated	42,66 67,68,71,88
bis-(2-ethoxy- ethyl)ether	$C_8H_{18}O_3$ $(C_2H_5OCH_2CH_2)_2O$	162	treated	76
ethylacetate	$C_4H_8O_2$ $H_3CCOOC_2H_5$	88	tube treated bottled	28 92 94

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
ethyl acetophenone	$C_{10}H_{12}O$ see E3	148	treated well	11
ethylamine	C_2H_7N $H_3CCH_2NH_2$	45	treated waste (USSR)	53, 41
ethylbenzene	C_8H_{10} $C_6H_5(C_2H_5)$	106	treated treated well rivers	20, 31, 59, 73, 76, 82, 83, 84, 92 10 2, 48
ethyl-N,N-diisobutyl- thiolcarbamate	(see sutan)			
ethyl ether	(see diethyl ether)			
*ethylglycolyl- ethylphthalate	$C_{14}H_{16}O_6$ see E4	280	tube	28
2-ethyl-n-hexane	C_8H_{18} see E5	114	treated	78
2-ethylhexanol	$C_8H_{18}O$ see E6	130	treated well tube rivers	11 28 2, 48
ethylindan	(see ethylindane)			
ethylindane	$C_{11}H_{14}$ see E7	146	treated	20
cis-2-ethyl-4- methyl-1,3- dioxolane	$C_6H_{12}O_2$ see E8	116	treated	77

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
trans-2-ethyl-4-methyl-1,3-dioxolane	$C_6H_{12}O_2$ see E9	116	treated	77
ethylmethyleketone	(see butanone)			
*p-ethylphenol	$C_8H_{10}O$ see E10	122	tube	28
ethylphthalyl-ethylglycollate	(see ethylglycollyethylphthalate)			
2-ethyltoluene	(see o-ethyltoluene)			
3-ethyltoluene	(see m-ethyltoluene)			
4-ethyltoluene	(see p-ethyltoluene)			
m-ethyltoluene	C_9H_{12} see E11	120	treated	20, 82, 92
o-ethyltoluene	C_9H_{12} see E12	120	treated river treated	20, 42 68, 82
p-ethyltoluene	C_9H_{12} see E13	120	treated river treated	20, 42 82
eucalyptol	(see 1,8-cineole)			
exo-2-camphanol	(see isoborneol)			

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
*fenac	$C_8H_5O_2Cl_3$ see F1	238	irriga.	18
*fenitrothion	$C_9H_{12}O_5NSP$ see F2	277	river	57
*fluoranthene	$C_{16}H_{10}$ see F3	202	rivers well	17, 25, 65 82
*formic acid	CH_2O_2 HCOOH	46	river	40
freon 11	(see trichlorofluoromethane)			
*fulvic acid	polymeric polymeric	900- 20,000	unk.	5
geosmin	$C_{12}H_{22}O$ see G1	182	lake treated	49 77
*glucose	$C_6H_{12}O_6$ see G2	180	lake	26
guaiacol	$C_7H_8O_2$ see G3	124	river treated	2 73, 84

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
HCB	(see hexachlorobenzene)			
HCE	(see heptachlorepoxyde)			
heptachlor	$C_{10}H_5Cl_7$ see H1	370	river treated	3,8,38 52,71,85
heptachlorepoxyde	$C_{10}H_5OCl_5$ see H2	386	river treated rain	8,9,38 52,71 63
1,2,3,4,5,7,7- heptachloro- norbornene	$C_7H_3Cl_7$ see H3	332	treated river river	42 3
heptachloro- norbornene isomer	$C_7H_3Cl_7$ see H4	332	treated river	42
heptadecane	$C_{17}H_{36}$ $H_3C(CH_2)_{15}CH_3$	240	treated	20
1-heptadecene	$C_{17}H_{34}$ $H_2C=CH(CH_2)_{14}CH_3$	238	treated	82
hexachlorane	(see hexachlorobenzene)			

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
hexachlorobenzene	C_6Cl_6 see H5	282	treated river treated	31 59,62,73,76
hexachloro-1,3- butadiene	C_4Cl_6 see H6	258	treated river	42
hexachlorocyclo- hexane	(see benzene hexachloride)			
hexachloroethane	C_2Cl_6 Cl_3C-CCl_3	234	treated river treated well treated	31,42 59,66 76
*1,2,3,4,6,6- hexachloro- norbornadiene	$C_7H_2Cl_6$ see H7	296	river	3
1,4,5,6,7,7- hexachloro-5- norbornene-2,3- dimethanolcyclicsulfite	(see endosulfan)			
hexachlorophene	$C_{13}H_6O_2Cl_6$ see H8	404	treated	4
hexadecane	$C_{16}H_{34}$ $H_3C(CH_2)_{14}CH_3$	226	treated river treated	55 20,67,71
C_2 hydrocarbon	C_2H_x unk	unk	treated	44
C_3 hydrocarbon	C_3H_x unk	unk	treated	44
C_4 hydrocarbon	C_4H_x unk	unk	treated	44

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
above C ₇ hydro- carbons	C ₇ H _x unk	unk	treated	44
>C ₁₀ hydrocarbons	>C ₁₀ H _x unk	unk	treated well	11
*C ₁₅ hydrocarbon	C ₁₅ H _x unk	unk	river	25
*C ₁₆₋₂₉ hydro- carbons	C ₁₆ H _x to C ₂₉ H _x unk	unk	river	25
2-hydroxyadipo- nitrile	C ₆ H ₈ ON ₂ see H9	124	treated	80
2-hydroxybiphenyl	(see o-phenylphenol)			
2-hydroxybornane	(see isoborneol)			
indan or indane	(see 2,3-dihydroindene)			
indene	C ₉ H ₈ see I1	116	treated well treated	10 20

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
*indeno(1,2,3-cd) pyrene	C ₂₂ H ₁₂ see I2	276	rivers	17,65,85
ionol	(see 2,6-di-t-butyl-p-cresol)			
isoacetophorone	(see isophorone)			
isoamylnitrile	(see 2-methylbutylnitrile)			
isoborneol	C ₁₀ H ₁₈ O see I3	154	treated river	59,73,84 2
isobutanal	(see 2-methylpropanal)			
isobutylnitrile	(see 2-methylpropylnitrile)			
isobutyraldehyde	(see 2-methylpropanal)			
*isobutyric acid	C ₄ H ₈ O ₂ H ₃ CCH(CH ₃)COOH	88	river	40
isocyanic acid	CHON HN=C=O	43	treated river	59,73,83,84 2
isodecane	C ₁₀ H ₂₂ see I4	142	treated	20,53,,
*isodrin	C ₁₂ H ₈ Cl ₆ see I5	362	river	3
isooctenone	C ₈ H ₁₄ O C ₈ H ₁₄ O unk. isomer	126	treated	20

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
isophorone	$C_9H_{14}O$ see I6	138	treated river	42,66
isopropanol	C_3H_8O $H_3CCH(OH)CH_3$	60	treated	75,77
1-isopropenyl-4- isopropylbenzene	$C_{12}H_{16}$ see I7	160	treated	59,73
isopropylbenzene	C_9H_{12} $C_6H_5(i-C_3H_7)$	120	treated river treated well	59,82,83,84 2 10
*isopropylphenol	$C_9H_{12}O$ see I8	136	tube	28
isoundecane	$C_{11}H_{24}$ see I9	156	treated	20
*isovaleric acid	$C_5H_{10}O_2$ see I10	102	river	40
*kerosene	C_xH_y unk	unk	river	37

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
*ketones	unk RCOR		river	36,37
lasso	(see alachlor)			
*lauric acid	$C_{12}H_{24}O_2$ $H_3C(CH_2)_{10}COOH$	200	tube	28
lignoceric acid	$C_{24}H_{48}O_2$ $H_3C(CH_2)_{22}COOH$	368	treated river	55 ✓
limonene	$C_{10}H_{16}$ see L1	136	treated river	42
lindane	$C_6H_6Cl_6$ see L2	288	river treated	33,38 52
p-menth-1-en- 8-ol	$C_{10}H_{18}O$ see M1	154	treated	59,73
methane	CH_4 CH_4	16	treated	43
methanol	CH_4O H_3COH	32	treated river treated	42,66 67

COMPOUND NAME	FORMULA STRUCTURE	Mwt.	WATER TYPE	REFERENCES
2-methoxybiphenyl	$C_{13}H_{12}O$ see M2	184	treated	59
o-methoxyphenol	(see guaiacol)			
*methylacetate	$C_3H_6O_2$ $H_3CCOOCH_3$	74	river	66
*methylamine	CH_5N H_3CNH_2	31	waste (USSR)	41, 85
methylbenzoate	$C_8H_8O_2$ $C_6H_5(COOCH_3)$	136	treated river	42
methylbenzo- thiazole	C_8H_7NS see M3	149	river treated	11 59
methylbenzo- thiophene	C_9H_8S see M4	148	treated	10
α -methylbenzyl- alcohol	(see methylphenylcarbinol)			
methylbiphenyl	$C_{13}H_{12}$ see M5	168	treated river	59, 73, 83, 84 2
methylbromide	(see bromomethane)			
3-methylbutanal	$C_5H_{10}O$ $H_3CCH(CH_3)CH_2CHO$	86	treated river treated well treated	42, 94 66 67
*2-methyl-2-butanol	$C_5H_{12}O$ $C_2H_5C(OH)(CH_3)CH_3$	88	well	77

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
3-methyl-2-butanone	$C_5H_{10}O$ $H_3CCH(CH_3)COCH_3$	86	treated river	66
2-methylbutyl- cyanide	(see 2-methylbutylnitrile)			
2-methylbutyl- nitrile	$C_6H_{11}N$ see M6	97	treated well	66
methylbutyraldehyde	(see 3-methylbutanal)			
methylchloride	CH_3Cl H_3CCl	50	treated river	59,67,73,83,84 2
methylcyclohexane	C_7H_{14} see M7	98	treated well	11
methylcyclopentane	C_6H_{12} see M8	84	treated	44
2-methyldecane	(see isoundecane)			
methyl-2,3- dihydroindene	$C_{10}H_{12}$ see M9	132	treated	10,20
*2-methyldioxalone?	$C_4H_8O_2$ see M18	88	well	75,77
methylenechloride	(see dichloromethane)			
2,2'-methylene-bis (3,4,6-trichloro- phenol)	(see hexachlorophene)			

COMPOUND NAME	FORMULA STRUCTURE	Mwt.	WATER TYPE	REFERENCES
methyl ester of lignoceric acid	(see methyltetracosanoate)			
methylether	C_2H_6O H_3COCH_3	46	treated river	66
methylethylketone	(see butanone)			
*2-methyl-5-ethyl- pyridine	$C_8H_{11}N$ see M10	121	river	48
methylformate	$C_2H_4O_2$ $HCCOOCH_3$	60	treated river	66
*3-methylfuran	C_5H_6O see M11	82	rain	51
methylin dan or methylin dane	(see methyl-2,3-dihydroindene)			
methylin denes	$C_{10}H_{10}$ see M12	130	treated well	10
*2-methylisoborneol	$C_{11}H_{20}O$ see M13	168	lake	49
methylisopropyl- ketone	(see 3-methyl-2-butanone)			
methyllignocerate	(see methyltetracosanoate)			
methylmethacrylate	$C_5H_8O_2$ $H_2C=C(CH_3)COOCH_3$	100	treated	68

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
methylnaphthalene	$C_{11}H_{10}$ see M14	142	treated well treated river	10,11 20,92 25
1-methylnaphthalene	$C_{11}H_{10}$ see M15	142	treated lake	82 56
2-methylnaphthalene	$C_{11}H_{10}$ see M16	142	treated lake	82 56
2-methylnonane	(see isodecane)			
methylpalmitate	$C_{17}H_{34}O_2$ $H_3C(CH_2)_{14}COOCH_3$	270	treated well treated	11 67,71,72
*3-methyl-3-pentanol	$C_6H_{14}O$ $C_2H_5C(OH)(CH_3)C_2H_5$	102	well	77
2-methylphenol	(see o-cresol)			
methylphenyl- carbinol	$C_8H_{10}O$ see M17	122	treated	48,78
2-methylpropanal	C_4H_8O $H_3CCH(CH_3)CHO$	72	treated well treated river treated	66 66 42,67
2-methylpropyl- nitrile	C_5H_9N $H_3CCH_2CH(CH_3)C\equiv N$	83	treated river	66
methylstearate	$C_{19}H_{38}O_2$ $H_3C(CH_2)_{16}COOCH_3$	298	treated	67,71,72,75,91

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
methylnonanoate	$C_{25}H_{50}O_2$ $H_3C(CH_2)_{22}COOCH_3$	382	treated	67,71
2-methylthiobenzo- thiazole	(see 2-thiomethylbenzothiazole)			
methylnaphthalene	(see methylbenzothiophene)			
*myristic acid	$C_{14}H_{28}O_2$ $H_3C(CH_2)_{12}COOH$	228	tube	28
methylantracene	$C_{15}H_{12}$ see M19	192	lake	56
naphthalene	$C_{10}H_8$ see N1	128	treated well river treated	10,11 25,48 20,53,76 82,92
*C ₃ naphthalene	$C_{13}H_{14}$ see N2	170	river	25
*C ₄ naphthalene	$C_{14}H_{16}$ see N3	184	river	25

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
*naphthylamine	$C_{10}H_9N$ see N4	143	river (Japan)	58
nicotine	$C_{10}H_{14}N_2$ see N5	162	treated well	66
*nitrilotriacetic acid	$C_6H_9O_6N$ see N6	191	river	34
nitroanisole	$C_7H_7O_3N$ $(NO_2)C_6H_4(OCH_3)$	153	treated raw	59 73
nitrobenzene	$C_6H_5O_2N$ $C_6H_5(NO_2)$	123	treated river	59,73,83,84 2
naphthyldichloromethane	$C_{11}H_8Cl_2$ see N8	210	treated river	94

COMPOUND NAME	FORMULA STRUCTURE	Mwt.	WATER TYPE	REFERENCES
*nitrochlorobenzene	$C_6H_4O_2NCl$ $(NO_2)C_6H_4(Cl)$	157	river	36
m-nitrochloro- benzene	(see m-chloronitrobenzene)			
nitromethane	CH_3O_2N H_3CNO_2	61	treated river	66
nitrotrichloro- methane	(see chloropicrin)			
nonadecane	$C_{19}H_{40}$ $H_3C(CH_2)_{17}CH_3$	268	treated	20
n-nonane	C_9H_{20} $H_3C(CH_2)_7CH_3$	128	treated river treated bottled	42 20, 53, 94
*p-nonylphenol	$C_{15}H_{24}O$ see N7	220	tube	28
NTA	(see nitrilotriacetic acid)			

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
octachlor	(see chlordanes)			
octachlorocamphene	(see toxaphene)			
octadecane	$C_{18}H_{38}$ $H_3C(CH_2)_{16}CH_3$	254	treated river treated	55, 94 20, 67, 71, 72
octane	C_8H_{18} $H_3C(CH_2)_6CH_3$	114	river treated	11 59
octylbutyl- fumarate	$C_{16}H_{28}O_4$ see 01	284	treated well	11
octylchloride	$C_8H_{17}Cl$ $H_3C(CH_2)_6CH_2Cl$	148	treated	53,
*organic acid	unk RCOOH		river	37
organophosphorus pesticides	unk unk		treated	46
octasulfur	S_8 S_8	256	treated	27
palmitic acid	$C_{16}H_{32}O_2$ $H_3C(CH_2)_{14}COOH$	256	treated river	55

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
paraldehyde	$C_6H_{12}O_3$ see P1	132	treated	20
pentachlorobi- phenyl	$C_{12}H_5Cl_5$ see P2	324	treated river treated	55 67,71
pentachloro- ethane	C_2HCl_5 Cl_2HCCCl_3	200	treated	92
pentachlorophenol	C_6HOCl_5 see P3	264	storage lake (Sweden) treated	13 50 4,12,90
pentachlorophenyl- methylether	$C_7H_3OCl_5$ see P4	278	treated	92
n-pentadecane	$C_{15}H_{32}$ $H_3C(CH_2)_{13}CH_3$	212	treated river treated	42 20
pentane	C_5H_{12} $H_3C(CH_2)_3CH_3$	72	river treated	11 59
pentanoic acid	(see valeric acid)			
pentanol	$C_5H_{12}O$ $H_3C(CH_2)_3CH_2OH$	88	treated	53,
pentene	C_5H_{10} $H_3CCH=CHCH_2CH_3$	70	treated	44
phenanthrene	$C_{14}H_{10}$ see P5	178	river treated	25 82

COMPOUND NAME	FORMULA STRUCTURE	Mwt.	WATER TYPE	REFERENCES
phenol	C_6H_6O $C_6H_5(OH)$	94	treated river	30, 85 61
phenolic compounds	unk unk		treated river	7 7
phenylacetic acid	$C_8H_8O_2$ $C_6H_5(CH_2COOH)$	136	treated river	66
phenylbenzoate	$C_{13}H_{10}O_2$ see P6	198	treated	67, 71, 72, 78
phenylether	$C_{12}H_{10}O$ see P7	170	river treated	36 20
phenylmethyl- carbinol	(see methylphenylcarbinol)			
o-phenylphenol	$C_{12}H_{10}O$ see P8	170	treated well	11
*phthalate	unk see P9		river	39
phthalic anhydride	$C_8H_4O_3$ see P10	148	tube treated	28 67, 71, 72, 78
piperidene	$C_5H_{11}N$ see P11	85	treated	53,
PNA	(see polynuclear aromatics)			
polyaromatic hydrocarbons	(see polynuclear aromatics)			

COMPOUND NAME	FORMULA STRUCTURE	Mwt.	WATER TYPE	REFERENCES
polychlorinated biphenyl	unk see Pl2		treated sea	32,82 22
polynuclear aromatics	unk unk		treated river	1,56 37
*propachlor	C ₁₁ H ₁₄ ONCl see Pl3	211	rivers	27
propanoic acid	(see propionic acid)			
propanol	C ₃ H ₈ O H ₃ CCH ₂ CH ₂ OH	60	treated	53, 75,77
propazine	C ₉ H ₁₆ N ₅ Cl see Pl4	229	treated	92
*propionic acid	C ₃ H ₆ O ₂ H ₃ CCH ₂ COOH	74	river	40
propylamine	C ₃ H ₉ N H ₃ CCH ₂ CH ₂ NH ₂	59	treated	53,
propylbenzene	C ₉ H ₁₂ C ₆ H ₅ (C ₃ H ₇)	120	treated	20,59,73,79
propyltoluene	C ₁₀ H ₁₄ (CH ₃)C ₆ H ₄ (C ₃ H ₇)	134	treated	20
pyrene	C ₁₆ H ₁₀ see Pl5	202	rivers treated	17,25,85 82

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
ramrod	(see propachlor)			
*ronnell	$C_8H_8O_3Cl_3$ SP see R1	320	rain	63
*C ₈ saturated alcohol	$C_8H_{18}O$ $C_8H_{17}OH$	130	tube	28
*silvex	$C_9H_7O_3Cl_3$ see S2	268	river	33
simazine	$C_7H_{12}N_5Cl$ see S1	201	treated	92
stearic acid	$C_{18}H_{36}O_2$ $H_3C(CH_2)_{16}COOH$	284	tube treated river	28 55
stryrene	C_8H_8 $C_6H_5(CH=CH_2)$	104	rivers treated	2,48 31,73,76,83,84

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
*substituted benzenes	unk $C_6H_5(R)$		river	37
*C ₃ substituted phenols	$C_9H_{12}O$ $(OH)C_6H_4(C_3H_7)$	136	tube	28
*sutan	$C_{11}H_{23}ONS$ see S3	217	river	27
*2,4,5-T	$C_8H_5O_3Cl_3$ see T1	254	rain	63
TDE	(see DDD)			
*tedion	$C_{12}H_6O_2Cl_4S$ see T2	354	river	35
o-terphenyl	$C_{18}H_{14}$ see T3	230	treated	20
1-terpineol	(see p-menth-1-en-8-ol)			
1,1,3,3-tetrachloro- acetone	$C_3H_2OCl_4$ $Cl_2CHCOCHCl_2$	194	treated	67,71,72,78

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
1,2,3,4-tetra- chlorobenzene	$C_6H_2Cl_4$ see T6	214	well	82
tetrachloro- biphenyl	$C_{12}H_6Cl_4$ see T7	290	treated river	55,67,71,72,78
tetrachloro- diphenylethane	(see DDD)			
tetrachloro- ethane	$C_2H_2Cl_4$ $Cl_2CHCHCl_2$	166	treated river treated	42 53,
1,1,1,2-tetra- chloroethane	$C_2H_2Cl_4$ Cl_3CCH_2Cl	166	treated	91
tetrachloro- ethylene	C_2Cl_4 $Cl_2C=CCl_2$	164	river treated river rain treated	2 42,66,94 51 16,31,44,59,67, 73,76,79,82,84, 86
tetrachloro- methane	(see carbon tetrachloride)			
tetrachlorophenol	$C_6H_2OCl_4$ $(OH)C_6H_1(Cl)_4$	230	treated	72
1,1,3,3-tetra- chloro-2-propanone	(see 1,1,3,3-tetrachloroacetone)			
n-tetradecane	$C_{14}H_{30}$ $H_3C(CH_2)_{12}CH_3$	198	treated river treated	42 20
tetradifon	(see tedion)			

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
1,2,3,4-tetra- hydronaphthalene	(see tetralin)			
*tetralin	$C_{10}H_{12}$ see T8	132	river	48
tetramethyl- benzene	$C_{10}H_{14}$ $C_6H_2(CH_3)_4$	134	treated	68
thianaphthene	(see benzothiophene)			
thiodan	(see endosufan)			
2-thiomethyl- benzothiazole	$C_8H_7NS_2$ see T9	181	river treated well	11 59,75 21
toluene	C_7H_8 $C_6H_5(CH_3)$	92	river treated river rain treated bottled	2,11,31 31,42,66,94 51 20,44,53,59,67, 73,75,76,79, 82,83,84 94
*toxaphene	$C_{10}H_{10}Cl_8$ unk	410	river	64
tributyl- phosphate	$C_{12}H_{27}O_4P$ see T11	266	treated well	27
*S,S,S-tributyl- phosphorotrithioate	$C_{12}H_{27}OS_3P$ see T12	314	waste	60
trichlorobenzene	$C_6H_3Cl_3$ $C_6H_3(Cl)_3$	180	treated river	20,53,75 24

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
1,2,3-trichloro- benzene	$C_6H_3Cl_3$ see T13	180	well	82
1,2,4-trichloro- benzene	$C_6H_3Cl_3$ see T14	180	treated	82
1,3,4-trichloro- benzene	(see 1,2,4-trichlorobenzene)			
1,3,5-trichloro- benzene	$C_6H_3Cl_3$ see T15	180	well	82
trichlorobiphenyl	$C_{12}H_7Cl_3$ see T16	256	treated river	55
1,1,1-trichloro- ethane	$C_2H_3Cl_3$ H_3C-CCl_3	132	treated river	66
1,1,2-trichloro- ethane	$C_2H_3Cl_3$ $ClCH_2-CHCl_2$	132	treated river treated well river treated	42, 94 59, 66 2 73, 84
1,1,2-trichloro- ethylene	C_2HCl_3 $Cl_2C=CHCl$	130	treated river treated	16, 42, 44, 66, 94 67, 69
trichloroethyl- phosphate	(see tris(chloroethylphosphate))			
trichlorofluoro- methane	CCl_3F CCl_3F	136	treated	53

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
trichloromethane	(see chloroform)			
2,4,6-trichlorophenol	$C_6H_3OCl_3$ see T17	196	treated	67,71,72,78
2,4,5-trichloro- phenoxypropionic acid	(see silvex)			
2,3,6-trichloro- phenylacetic acid	(see fenac)			
1,1,1-trichloro- propane	$C_3H_5Cl_3$ $H_3CCH_2CCl_3$	146	treated	92
1,2,3-trichloro- propane	$C_3H_5Cl_3$ $ClCH_2CHClCH_2Cl$	146	treated	92
n-tridecane	$C_{13}H_{28}$ $H_3C(CH_2)_{11}CH_3$	184	treated river	42
triglycodichloride	$C_6H_{12}O_2Cl_2$ $ClCH_2CH_2OCH_2CH_2OCH_2CH_2Cl$	186	treated	11,59,66
trimethylbenzene	C_9H_{12} $C_6H_3(CH_3)_3$	120	treated	20,68,79,92
1,2,3-trimethyl- benzene	C_9H_{12} see T19	120	treated	20,82
1,2,4-trimethyl- benzene	C_9H_{12} see T20	120	treated	20,82

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
1,3,5-trimethyl- benzene	C_9H_{12} see T21	120	treated	82
3,5,5-trimethyl- bicyclo(4,1,0) heptene-2-one	$C_{10}H_{14}O$ see T22	150	treated	81
3,5,5-trimethyl- 2-cyclohexen-1- one	(see isophorone)			
trimethylisocyanurate	$C_6H_9O_3N_3$ see T23	171	treated river	66,92
trimethyltrioxo- hexahydrotriazine	(see trimethylisocyanurate)			
triphenylphosphate	$C_{18}H_{15}O_4P$ see T24	326	treated river	42
trolene	(see ronnell)			
tetrahydrofuran	C_4H_8O see T25	72	treated river	94
n-undecane	$C_{11}H_{24}$ $H_3C(CH_2)_9CH_3$	156	treated river treated bottled	42 20 94

COMPOUND NAME	FORMULA STRUCTURE	MWt.	WATER TYPE	REFERENCES
undecane isomer	$C_{11}H_{24}$ $C_{11}H_{24}$	156	treated river	42
*valeric acid	$C_5H_{10}O_2$ $H_3C(CH_2)_3COOH$	102	river	40
*veratrole	$C_8H_{10}O_2$ see VI	138	river	2
veratrole- 1,2-isomer	(see dimethoxybenzene)			
veronal	(see barbital)			
vinylbenzene	(see styrene)			
vinylchloride	C_2H_3Cl $H_2C=CHCl$	62	treated	66
vinylidene- chloride	(see 1,1-dichloroethylene)			
m-xylene	(see 1,3-dimethylbenzene)			
o-xylene	(see 1,2-dimethylbenzene)			
p-xylene	(see 1,4-dimethylbenzene)			

*These chemicals have not been found in drinking water but are potential contaminants since they have been found in other waters as noted.

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Appendix I

Structural Formulas of Organic Compounds (alpha numeric as they occur in Table I)

A-1

A-2

A-3

A-4

A-5

A-6

A-7

A-8

A-9

A-10

A-11

A-12

A-13

E-1

E-2

E-3

E-4

E-5

E-6

E-7

E-8

E-9

E-10

E-11

E-12

E-13

F-1

F-2

F-3

G-1

G-2

G-3

H-1

H-2

H-3

H-4

H-5

H-6

H-7

H-8

H-9

I-1

I-2

I-3

I-4

I-5

I-6

I-7

I-8

I-9

I-10

P-1

P-2

P-3

P-4

P-5

P-6

P-7

P-8

P-9

P-10

P-11

P-12

P-13

P-14

P-15

T-21

T-22

T-23

T-24

T-25

V-1