

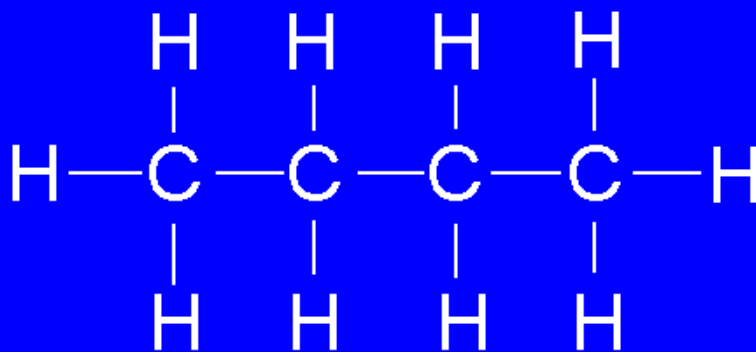
**Figure 5-1.** Two- and three-dimensional structural formulas for dichloromethane,  $\text{CH}_2\text{Cl}_2$ . In a two-dimensional representation, single, normal-weight lines indicate bonds extending away from the viewer and arrows indicate bonds extending toward the viewer.

# Butane

Condensed structural formula



Structural formula

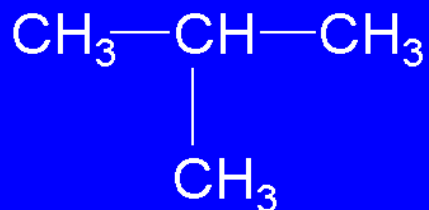


**Figure 5-2.** Relationship between the condensed structural formula and the structural formula of butane.

## Butane

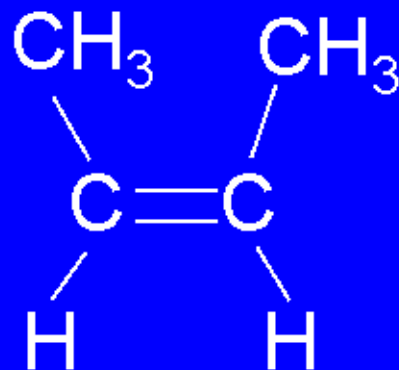


## 2-Methylpropane

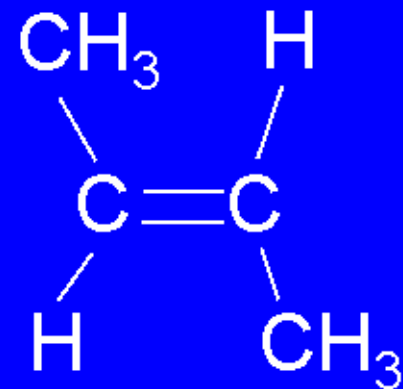


**Figure 5-3.** Isomers of  $\text{C}_4\text{H}_{10}$ . Both butane and 2-methylpropane have the same number of C and H atoms, but 2-methylpropane has a branched chain.

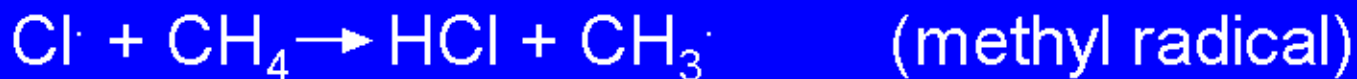
**Figure 5-4.** Examples of geometric isomers, *cis*-2-butene and *trans*-2-butene. In the first isomer, the two substituent groups are on the same side of the double bond. In the second isomer, the two substituent groups are on opposite sides of the double bond.



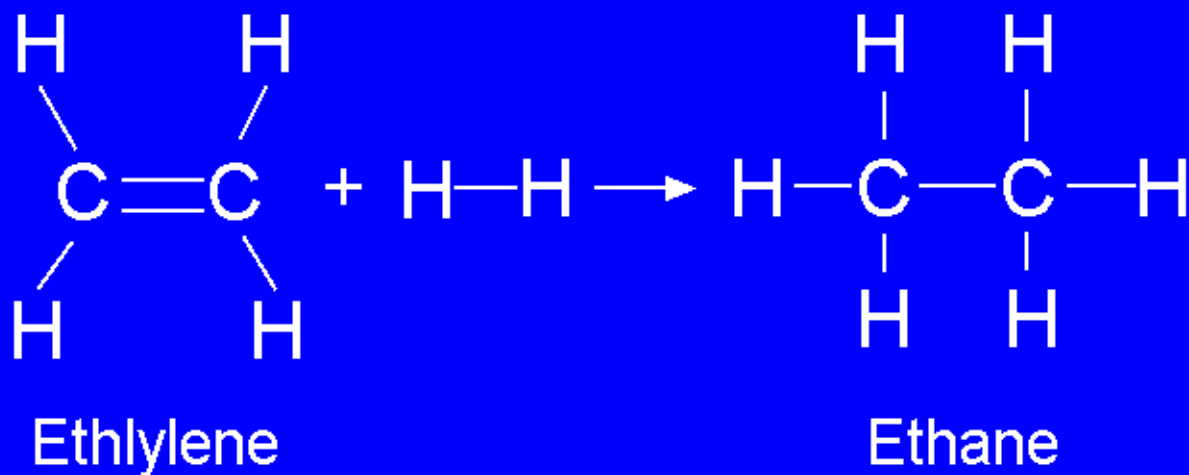
*cis*-2-butene



*trans*-2-butene



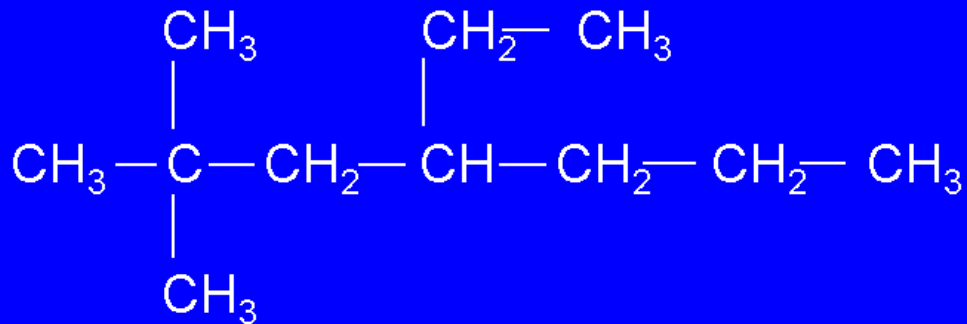
**Figure 5-5.** Example of a substitution reaction in which a hydrogen atom is replaced by a chlorine atom to produce chloromethane.



**Figure 5-6.** Example of an addition reaction in which hydrogen is added to ethylene to produce ethane (a hydrogenation reaction).

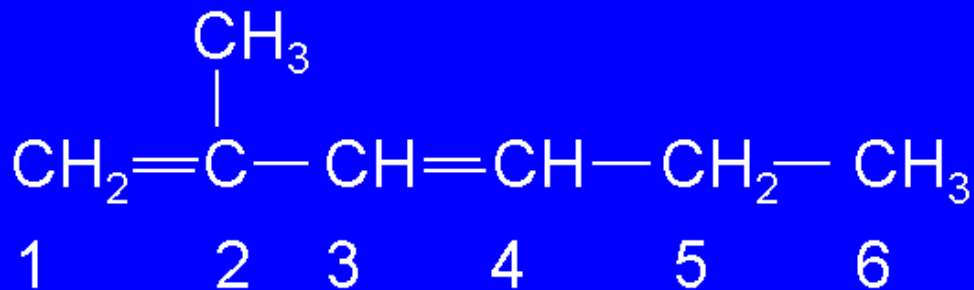
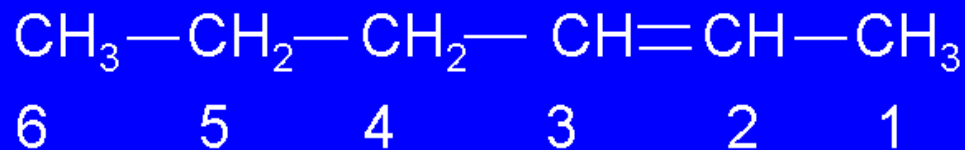
**Table 5-1. Prefixes for the number of carbon atoms**

# C	Prefix	# C	Prefix	# C	Prefix
1	Meth	11	Undec	21	Henicos
2	Eth	12	Dodec	22	Docos
3	Prop	13	Tridec	23	Tricos
4	But	14	Tetradec	24	Tetracos
5	Pent	15	Pentadec	25	Pentacos
6	Hex	16	Hexadec	26	Hexacos
7	Hept	17	Heptadec	27	Heptacos
8	Oct	18	Octadec	28	Octacos
9	Non	19	Nonadec	29	Nonacos
10	Dec	20	Eicos	30	Triacont



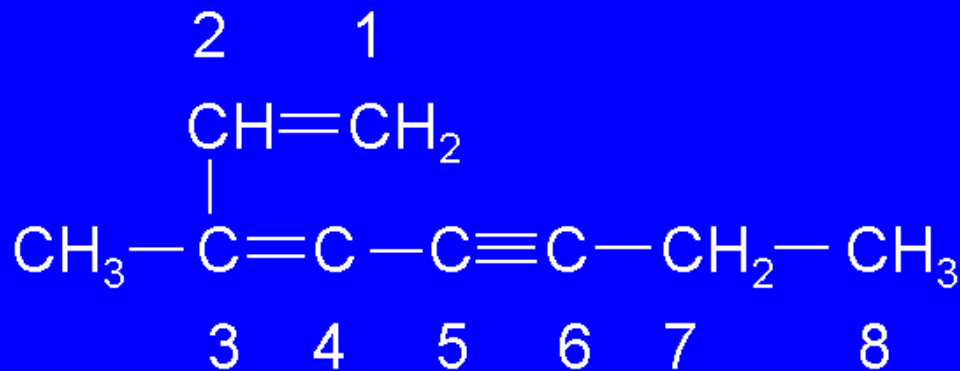
**Figure 5-7.** Condensed structural formula for the alkane 4-ethyl-2,2-dimethylheptane.

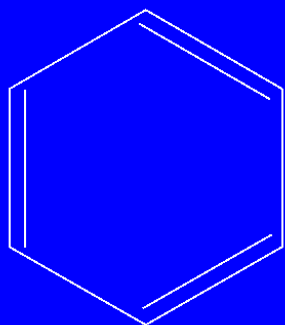
**Figure 5-8.** Condensed structural formula for 2-hexene.



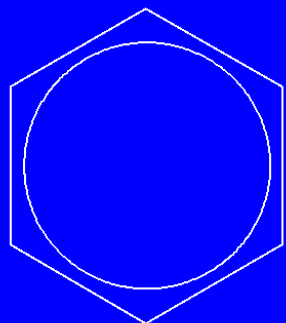
**Figure 5-9.** Condensed structural formula for 2-methyl-1,3-hexdiene.

**Figure 5-10.** Condensed structural formula for 3-methyl-1,3-octdien-5-yne.



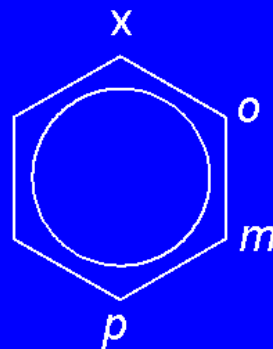


Benzene ring shown as alternating single and double bonds



Benzene ring shown as a ring of delocalized electrons

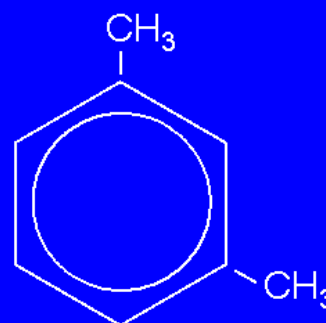
**Figure 5-11.** Representations of the benzene ring found in the literature.



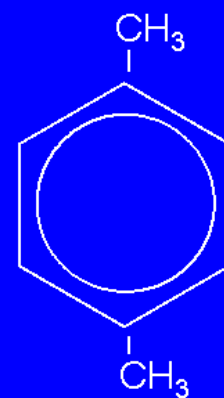
x is an substituent  
o = ortho position  
m = meta position  
p = para position



1,2-dimethylbenzene  
*o*-xylene

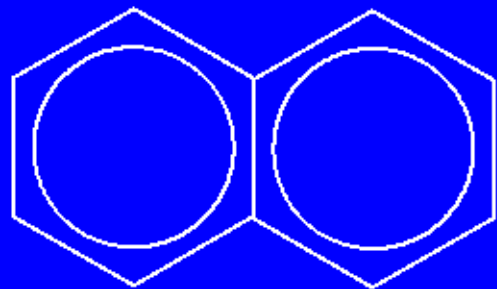


1,3-dimethylbenzene  
*m*-xylene

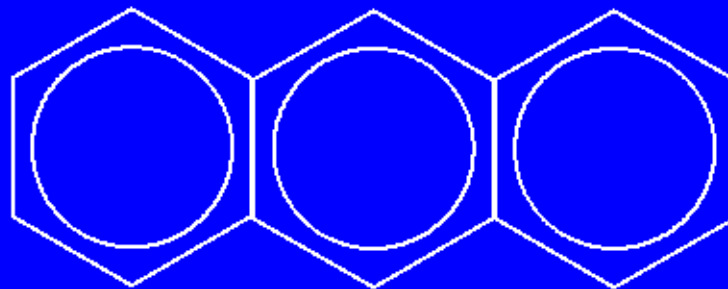


1,4-dimethylbenzene  
*p*-xylene

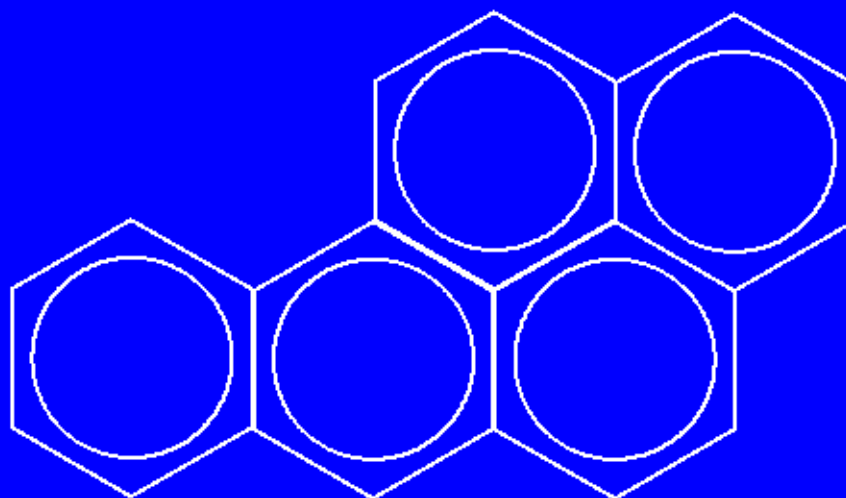
**Figure 5-12.** Illustration of the naming conventions for the benzene ring using attached methyl groups. Note that while now shown on the diagram, the other sites are occupied by hydrogen atoms.



Napthalene



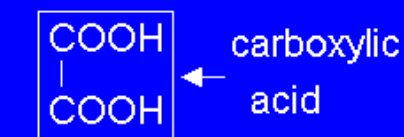
Anthracene



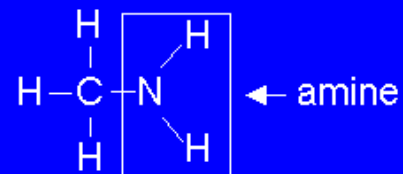
Benzo(a)pyrene

**Figure 5-13.** Examples of polycyclic aromatic hydrocarbons (PAHs) including the known carcinogen benzo(a)pyrene. Where the benzene rings do not share edges, hydrogen atoms are attached to the carbon atoms.

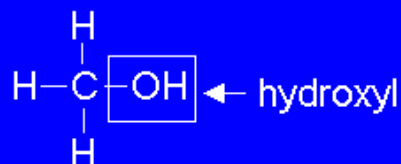
**Figure 5-14.** Examples of important functional groups. For each molecule the functional group is enclosed in a box and the name of the group is indicated by the arrow. The name of the compound is listed under each molecule.



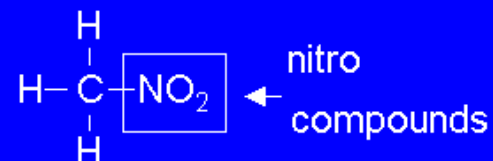
Oxalic acid



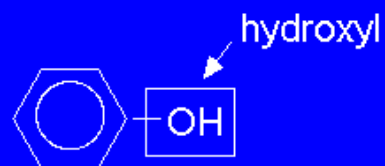
Methylamine



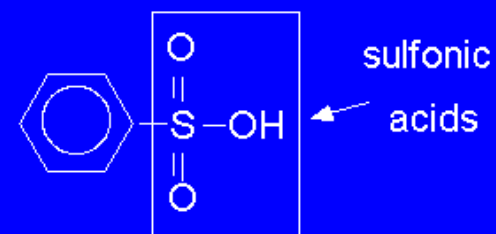
Methanol



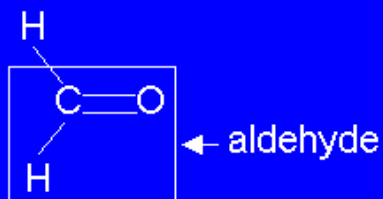
Nitromethane



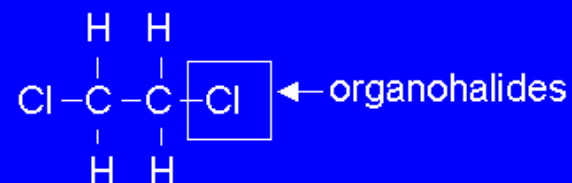
Phenol



Benzenesulfonic acid



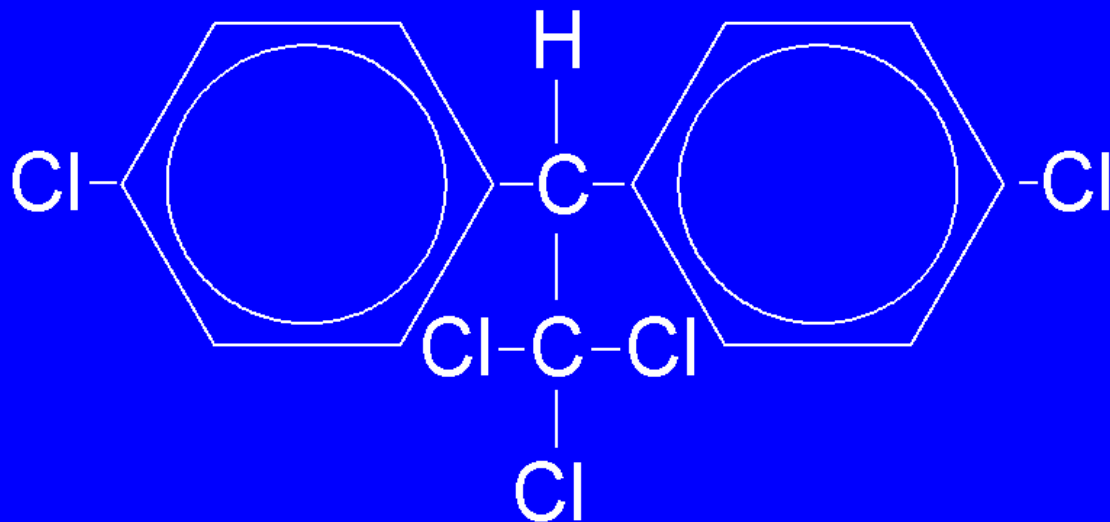
Formaldehyde



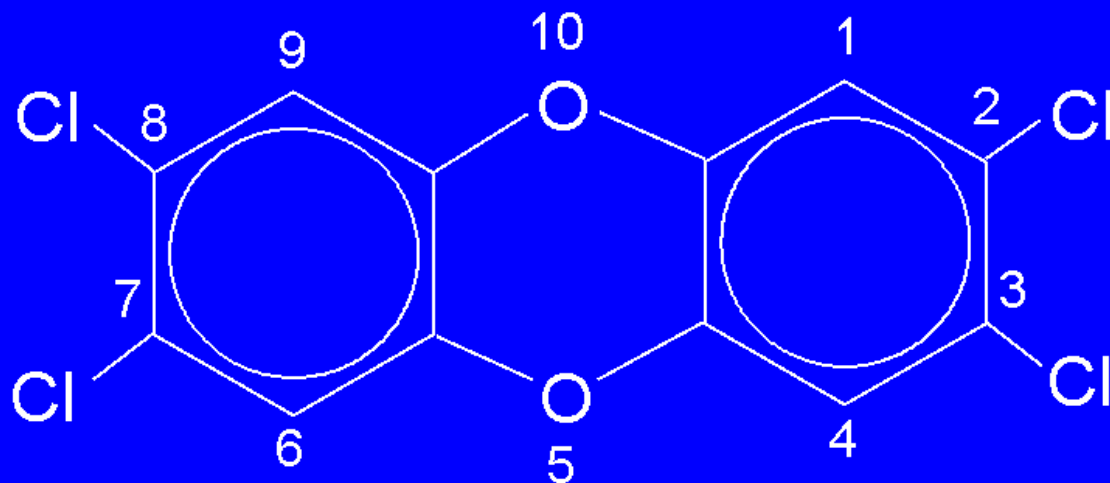
1,2-Dichloroethane

**Table 5-2. Examples of halogenated hydrocarbons**

Name	Formula	Name	Formula
Chloromethane	CH <sub>3</sub> Cl	1,1,2,2-Tetrachloroethane	Cl <sub>2</sub> CH-CHCl <sub>2</sub>
Bromomethane	CH <sub>3</sub> Br	1,1,1,2-Tetrachloroethane	Cl <sub>3</sub> C-CH <sub>2</sub> Cl
Dichloromethane	CH <sub>2</sub> Cl <sub>2</sub>	Pentachloroethane	Cl <sub>3</sub> C-CHCl <sub>2</sub>
Trichloromethane	CHCl <sub>3</sub>	Hexachloroethane	Cl <sub>3</sub> C-CCl <sub>3</sub>
Tetrachloromethane	CCl <sub>4</sub>	2-Chloropropane	CH <sub>3</sub> -CHCl-CH <sub>3</sub>
Bromodichloromethane	CHCl <sub>2</sub> Br	1,2-Dibromo-3-chloropropane	BrCH <sub>2</sub> -BrCH-CH <sub>2</sub> Cl
Trichlorofluoromethane	CCl <sub>3</sub> F	Chloroethene	CH <sub>2</sub> =CHCl
Chlorodifluoromethane	CHClF <sub>2</sub>	1,1-Dichloroethene	CH <sub>2</sub> =CCl <sub>2</sub>
Dichlorodifluoromethane	CCl <sub>2</sub> F <sub>2</sub>	Trichloroethene	ClCH=CCl <sub>2</sub>
Chloroethane	CH <sub>3</sub> -CH <sub>2</sub> Cl	Tetrachloroethene	Cl <sub>2</sub> C=CCl <sub>2</sub>
1,2-Dichloroethane	ClCH <sub>2</sub> -CH <sub>2</sub> Cl	1-Chloropropene	ClCH=CH-CH <sub>3</sub>
1,1,1-Trichloroethane	CH <sub>3</sub> -CCl <sub>3</sub>	1,3-Dichloropropene	ClCH=CH-CH <sub>2</sub> Cl



**Figure 5-15.** Structure of DDT. The molecule consists of two benzene rings joined by a chlorinated ethane group. Each ring has a Cl atom substituting for a H atom. The IUPAC name for this molecule would be dichlorodiphenyltrichloroethane.



**Figure 5-16.** Structure of 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (TCDD). The rings are numbered as shown. Note that the chlorine atoms occur in positions 2, 3, 7, and 8. The tetra prefix indicates that there are four chlorine atoms.

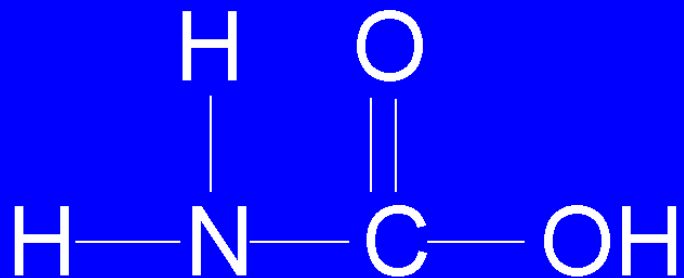
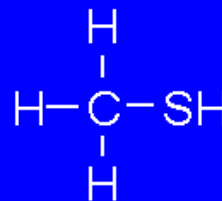


Figure 5-17. Carbamic acid.

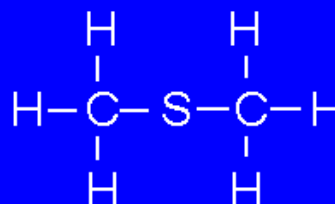
**Figure 5-18.** Examples of organosulfates. Thiols – methanethiol and benzenethiol, sulfides – dimethyl sulfide and dimethyl disulfide, thiourea – thiourea, sulfoxides – dimethylsulfoxide, sulfonic acids – benzenesulfonic acid, sulfates – methylsulfuric acid.



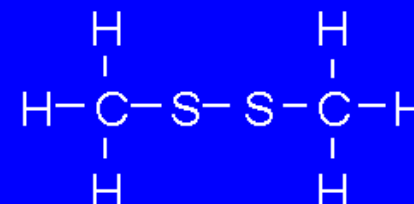
Methanethiol



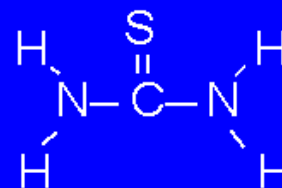
Benzenethiol



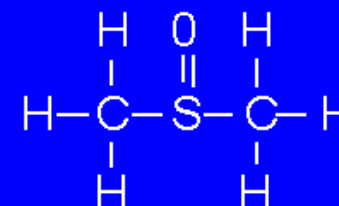
Dimethyl sulfide



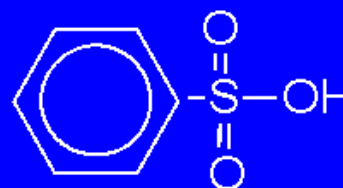
Dimethyl disulfide



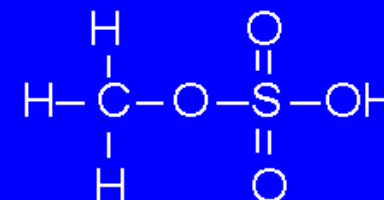
Thiourea



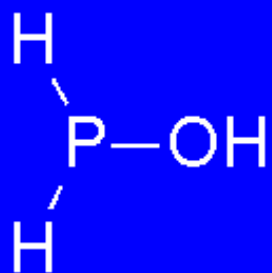
Dimethylsulfoxide (DMSO)



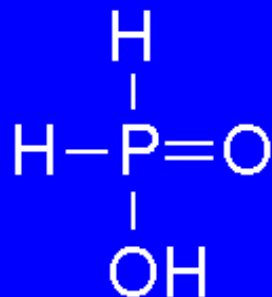
Benzenesulfonic acid



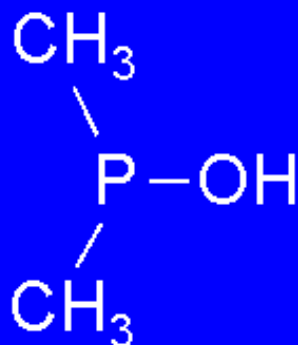
Methylsulfuric acid



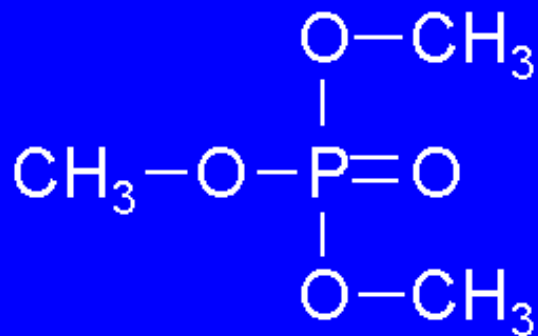
Phosphinous acid



Phosphinic acid

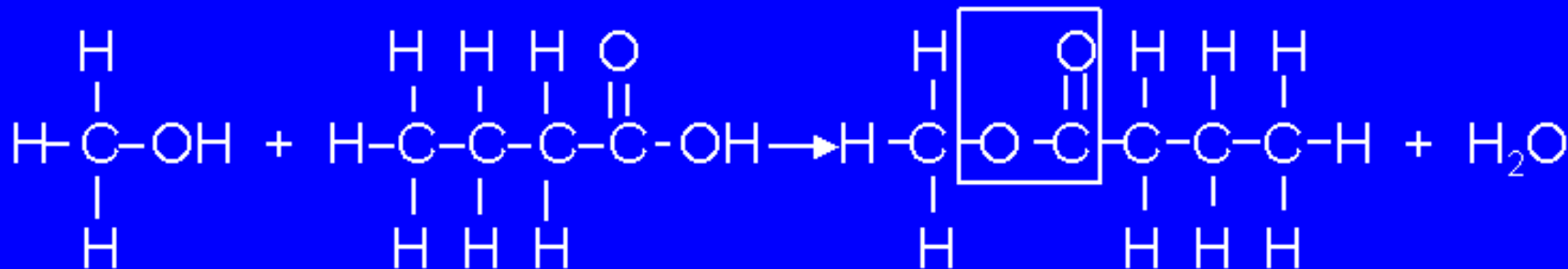


Dimethylphosphinic  
acid



Trimethyl phosphate

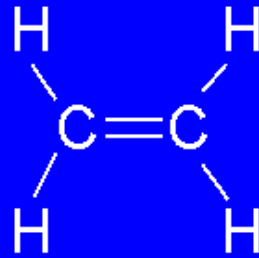
**Figure 5-19.** Examples of organophosphorus compounds. See text for description of naming conventions.



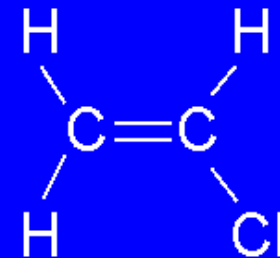
Methanol + Butanoic acid  $\longrightarrow$  Methyl butanoate

**Figure 5-20.** Condensation reaction between an alcohol (methanol) and a carboxylic acid (butanoic acid) to form an ester (methyl butanoate). Note that water is expelled during this reaction. The ester functional group is enclosed by the box.

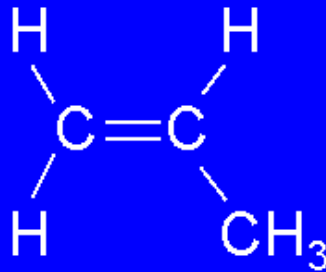
**Figure 5-21.** Examples of monomers used to build the common synthetic polymers. See text for examples of the uses of each synthetic polymer.



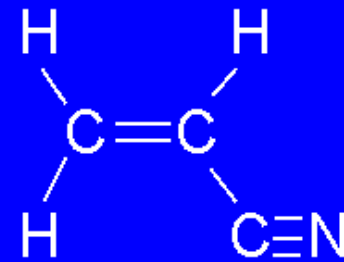
Ethylene



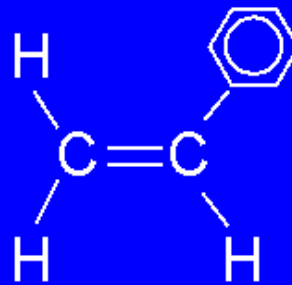
Vinyl chloride



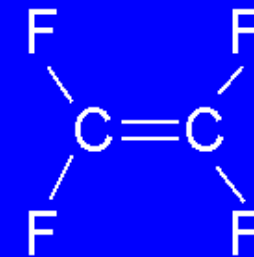
Propylene



Acrylonitrile

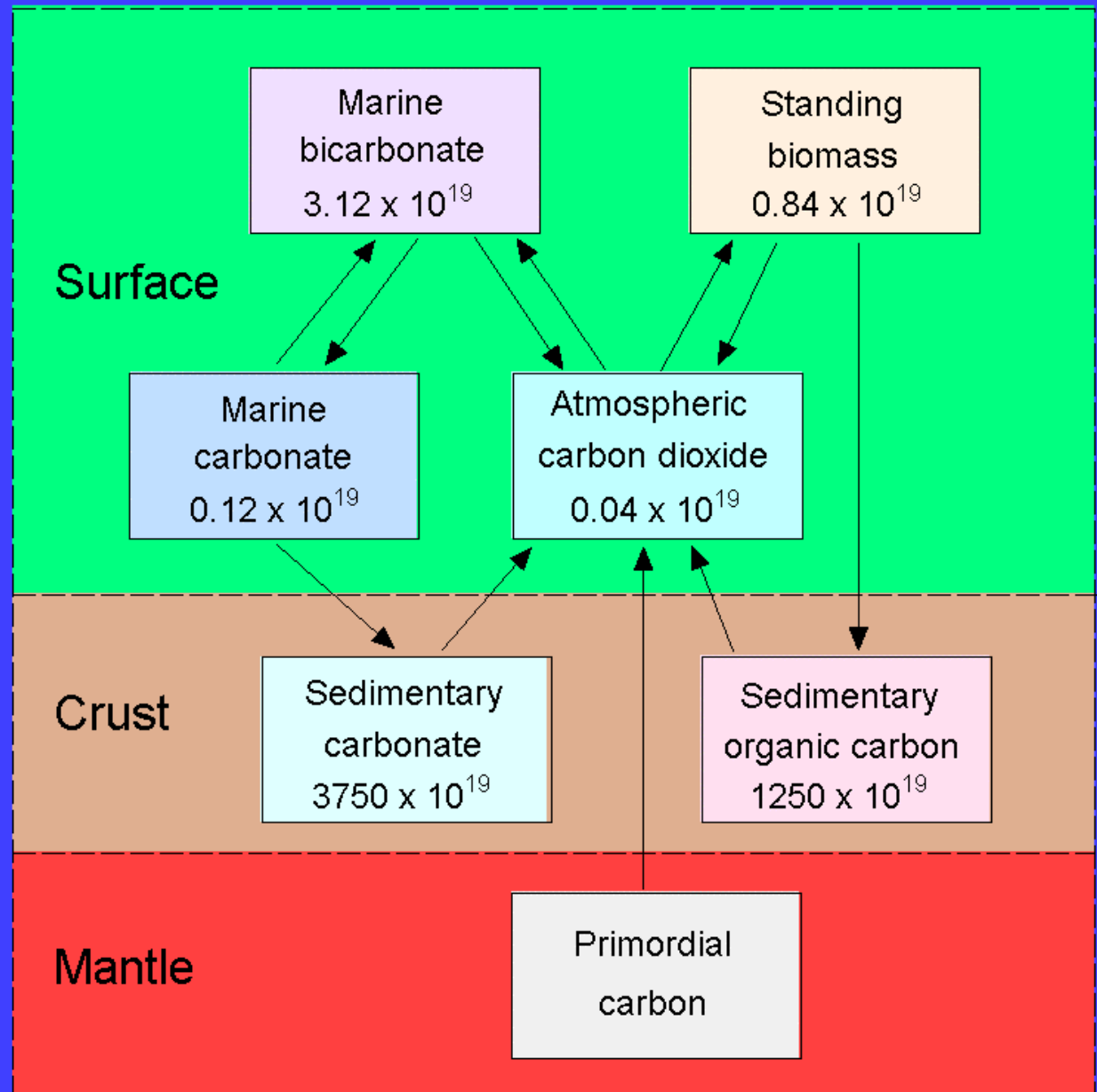


Styrene

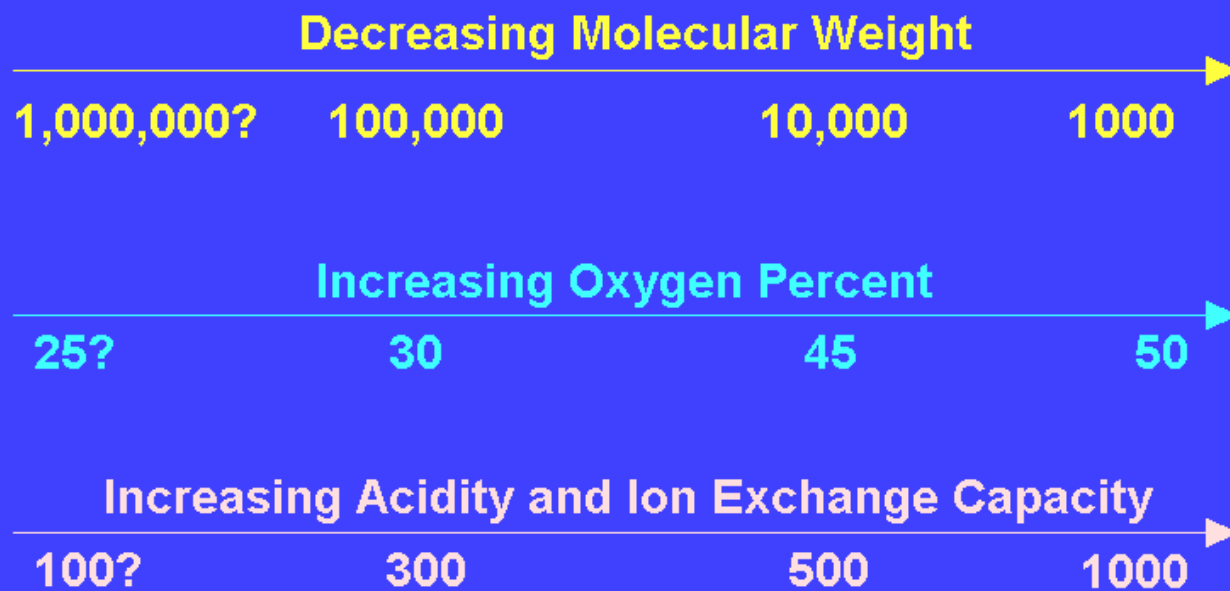
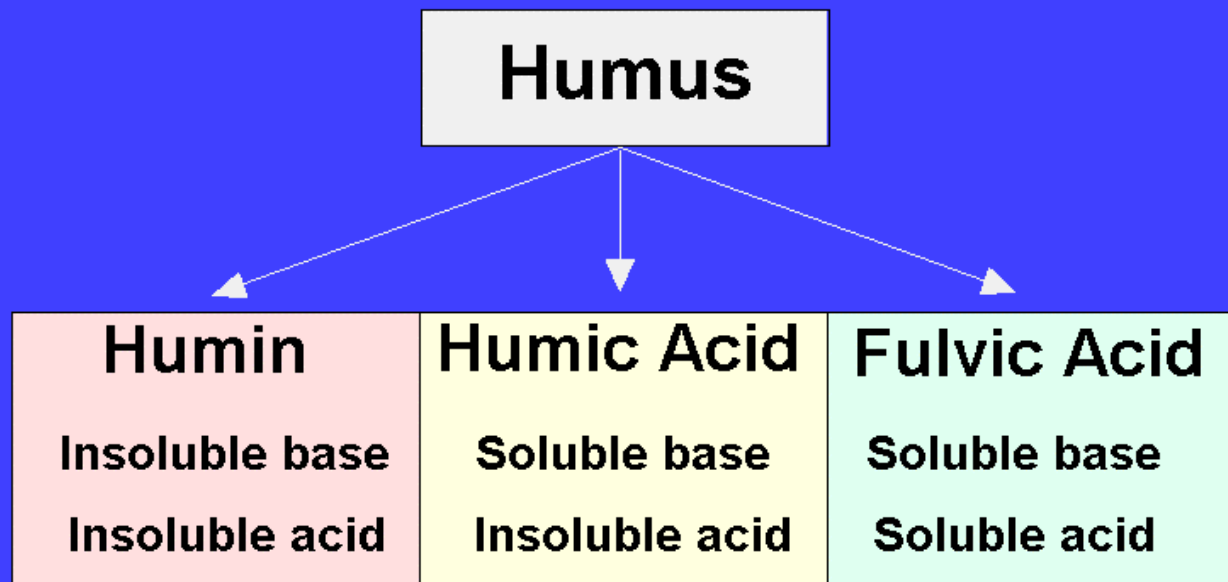


Tetrafluoroethylene

**Figure 5-22.** Major carbon reservoirs and interactions between these reservoirs. Carbon concentrations are in grams of carbon. Data from Schidlowski (1988).



**Figure 5-23.** Types of humic substances and general characteristics. Note that the distinction between the types of substances is based on their solubility in acids and bases. After Oades (1989).



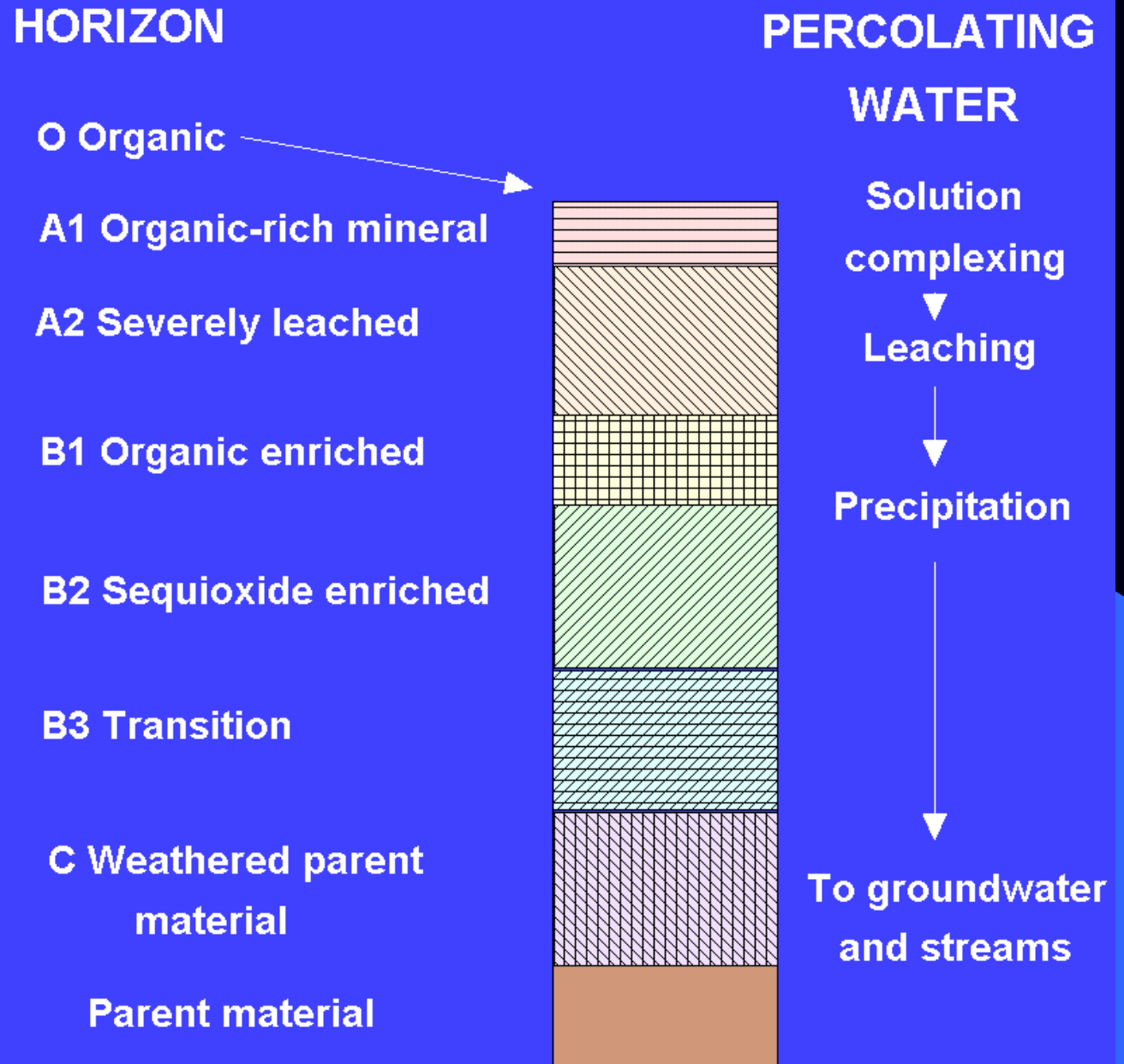
**Table 5-3. Elemental compositions, atomic ratios and atomic weights for soil humic and fulvic acids**

	Humic Acids	Fulvic Acids
Carbon (wt. %)	53.6 - 58.7	40.7 - 50.6
Hydrogen (wt. %)	3.2 - 6.2	3.8 - 7.0
Nitrogen (wt. %)	0.8 - 5.5	0.9 - 3.3
Oxygen (wt. %)	32.8 - 38.3	39.7 - 49.8
Sulfur (wt.%)	0.1 - 1.5	0.1 - 3.6
Mol. Wt. (Daltons)	2000 - 5000	500 - 2000
H/C (atomic)	~0.8	~1.3
O/C (atomic)	~0.5	~0.8

**Table 5-4. Compositon of humic substances in various environments**

	Soil	Ground water	Surface water	Lake sediments	Sea water	Marine sediments
Aromatic hydrocarbons	20 - 35%	-	17 - 30%	<15%	<15%	<15%
H/C	0.5 - 1.0	0.7 - 1.2	0.7 - 1.1	1.0-1.6	1.6	1.0 - 1.5
Molecular weights	$10^3 - 10^6$	$500 - 10^4$	$<10^4$	$10^3 - 10^6$	$<10^3$	-

**Figure 5-24.** Generalized soil profile for a spodosol. After Stevenson (1985). From HUMUS CHEMISTRY, GENESIS, COMPOSITION, REACTIONS by Stevenson. Copyright 1994. This material is used by permission of John Wiley & Sons, Inc.



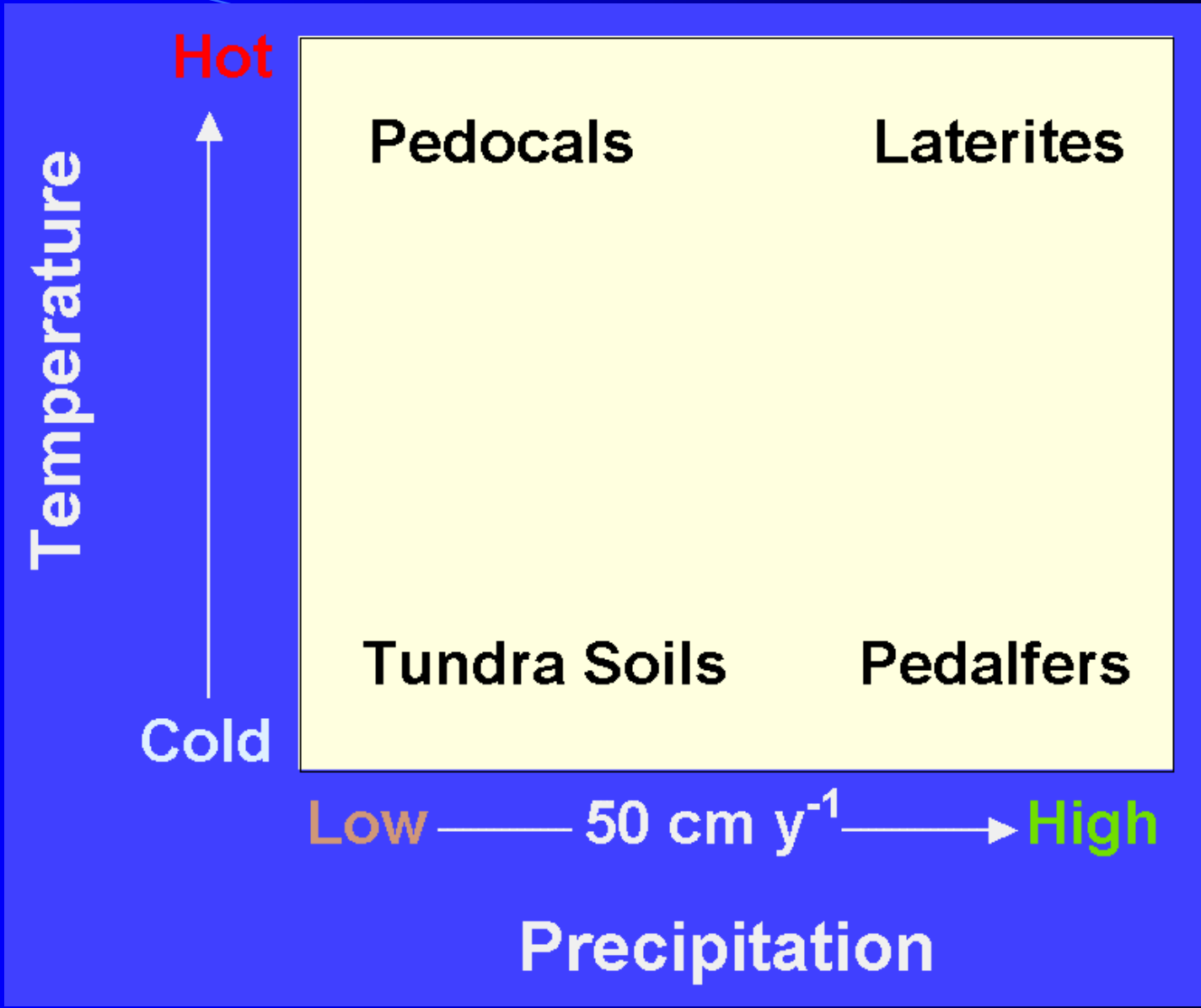
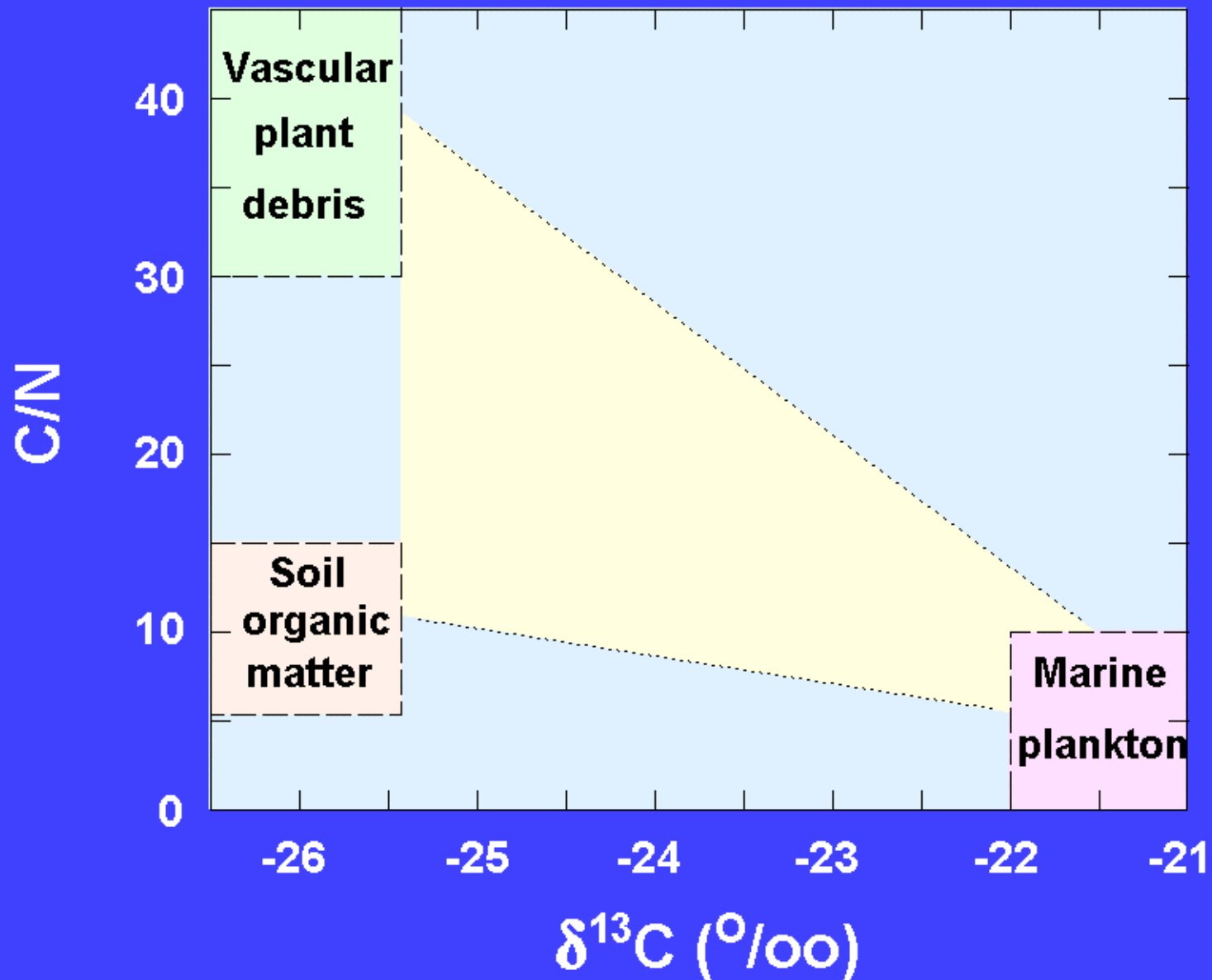


Figure 5-25. Soil types as a function of the climate variables temperature and precipitation.

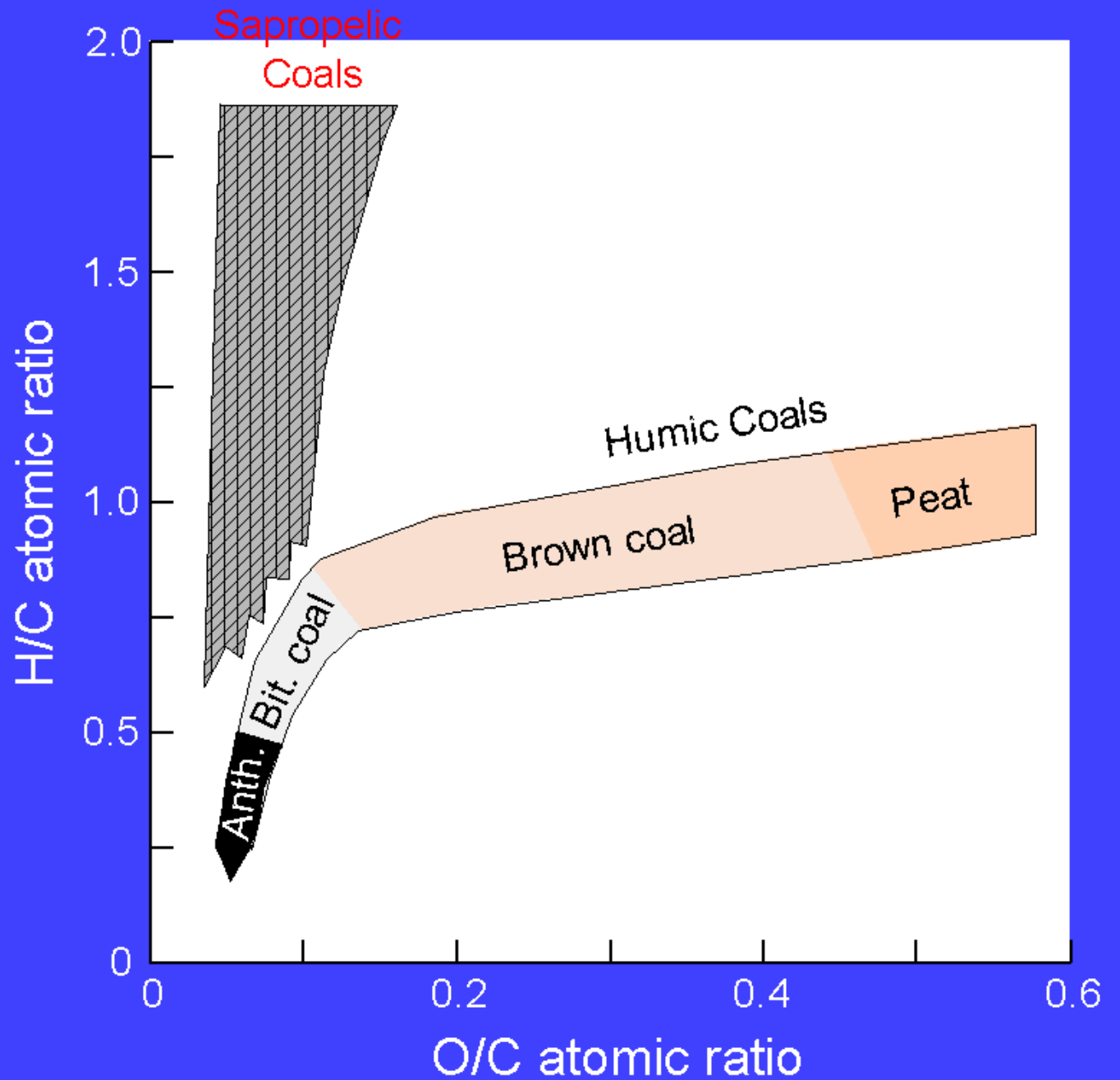
**Table 5-5. Soil Classification**

Soil type	Characteristics and climatic conditions
Oxisols	Extensive alteration of silicate minerals to form clays, such as kaolinite, and iron oxides; wet equatorial regions
Calcisols	Precipitation of calcium carbonate as nodules and layers; hot dry regions
Gypsisols	Calcium sulfate forms in soil as gypsum or anhydrite; very arid regions
Gleysols	Waterlogged soils with poor drainage and reducing conditions; temperate and polar regions
Argillisols	Layers and grain coating of clay are common; wet mid-latitude regions
Spodosols	Grain coatings of organic material and iron oxides; wet mid-latitude regions
Vertisols	Poorly developed layering but strong vertical structures due to repeated desiccation of expandable clays; relatively dry regions
Histisols	High concentrations of organic material forming peat layers; moist temperate regions and occasionally humid equatorial regions
Protosols	Poorly developed soils; most common in polar regions but can occur anywhere



**Figure 5-26.** Atomic C/N versus  $\delta^{13}\text{C}$  for various reservoirs of organic carbon. Mixtures of the three end members lie within the field defined by the dashed lines. Modified from Hedges and Oakes (1997).

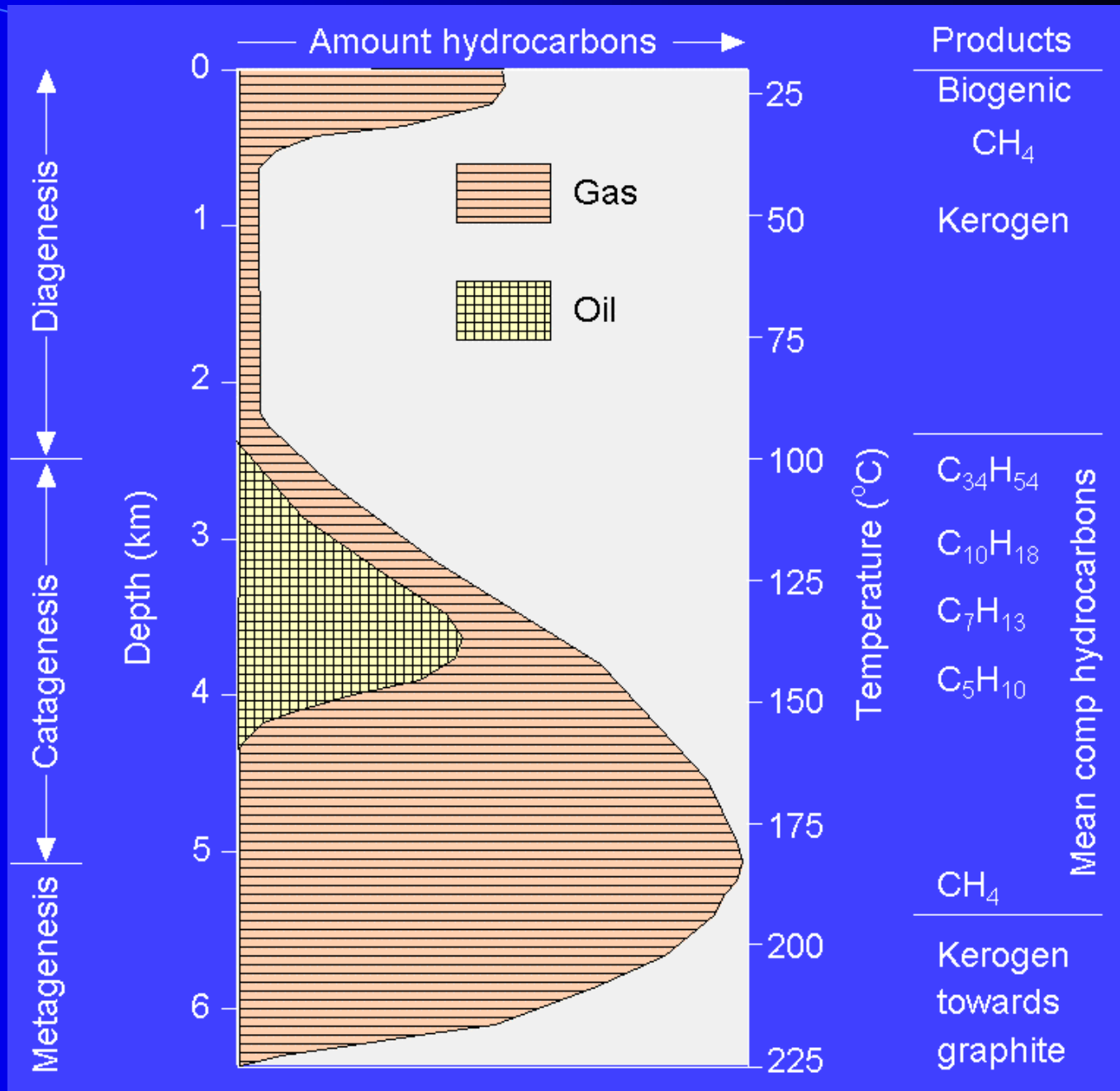
**Figure 5-27.** Van Krevelen (1963) diagram indicating the changes in hydrogen, oxygen, and carbon during the coalification process. After Killips and Killips (1993).



**Table 5-6. Concentration ranges in coal for some elements of environmental interest**

Element	Concentration range (ppm)	Element	Concentration range (ppm)
Sc	0.6 - 10.3	As	0.7 - 31
V	6 - 109	Se	0.4 - 3.3
Cr	2.6 - 25.4	Sb	0.1 - 7.3
Co	1.1 - 24.1	W	0.2 - 1.3
Ni	2 - 50	Pb	3 - 20
Cu	6 - 54	Th	0.5 - 3.7
Zn	3 - 65	U	0.2 - 3.8

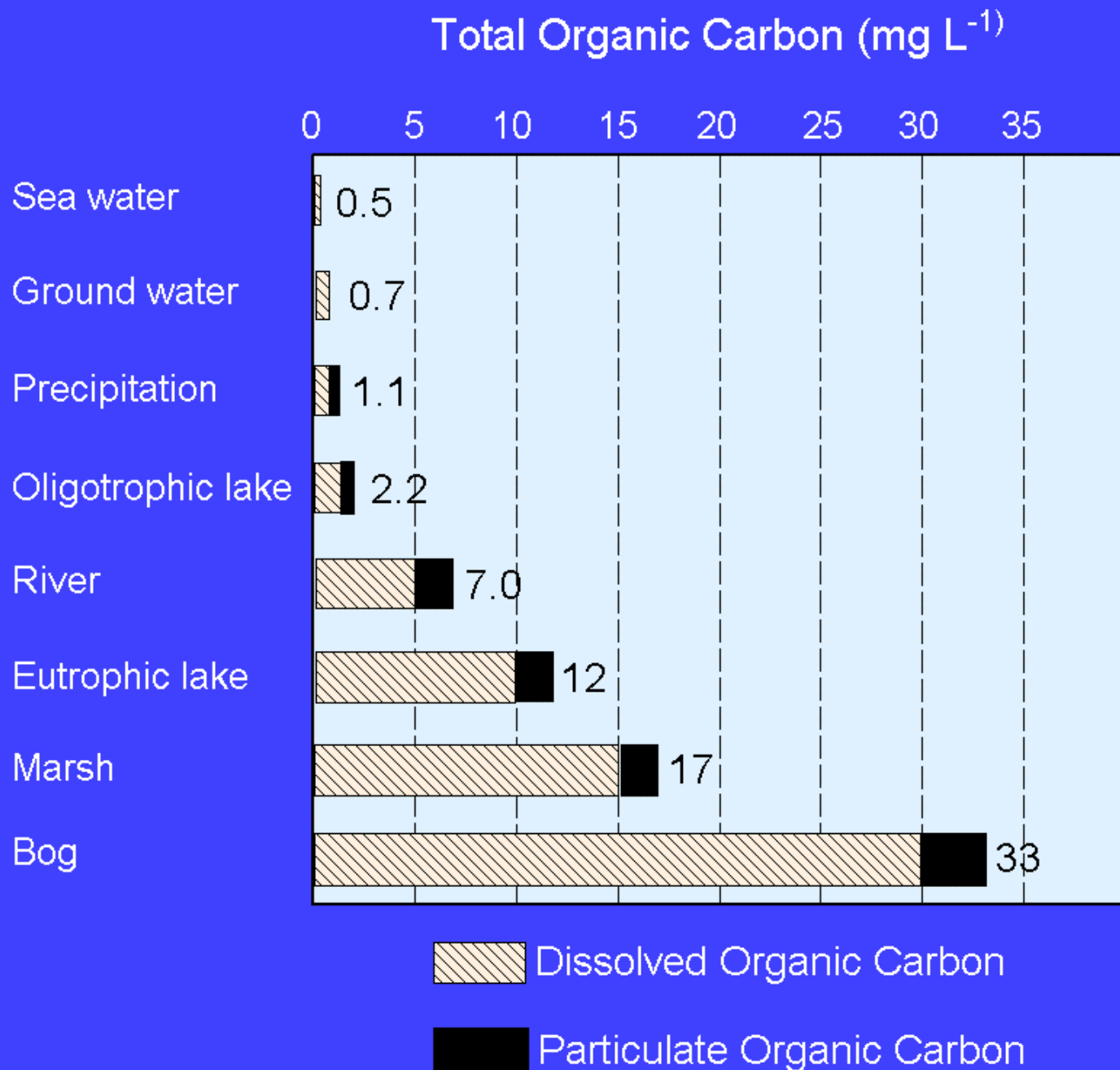
**Figure 5-28.** Schematic representation of production of petroleum from a typical reservoir rock assuming an average geothermal gradient. Note the narrow P-T range over which oil is produced (called the *petroleum window*). With increasing temperature, the size of the mean hydrocarbon molecule decreases. During catagenesis, hydrocarbon chains break off and are expelled from the kerogen. During metagenesis, only methane is released. Modified from Killops and Killops (1993).



**Table 5-7. Elemental composition of crude oil**

Element	Abundance
	<i>In wt. %</i>
C	82.2-87.1
H	11.8-14.7
S	0.1-5.5
O	0.1-4.5
N	0.1-4.5
Others	<0.1
	<i>In ppm</i>
Ni	0.3-200
V	0.3-1000

**Figure 5-29.** Average organic carbon concentrations for various aquatic systems. Note that the actual range in TOC can be substantial and depends on a variety of factors. See text. Taken from Thurman (1985a).

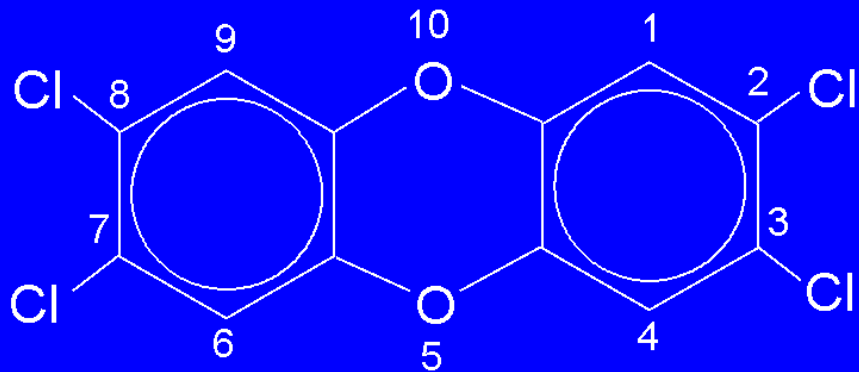


**Table 5-8. Median concentrations of organic carbon in various types of aquifers**

Aquifer	DOC (mg C L <sup>-1</sup> )
Sand and gravel	0.7
Limestone	0.7
Sandstone	0.7
Igneous	0.5
Oil shale	3
Humic colored	10
Petroleum associated	100

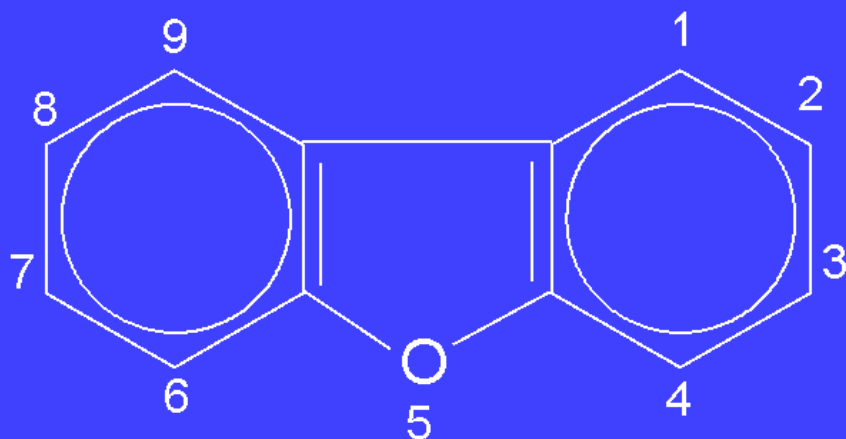
**Table 5-9. Data for selected pesticides**

Pesticide	Solubility in H <sub>2</sub> O (mg kg <sup>-1</sup> )	LD <sub>50</sub> (mg kg <sup>-1</sup> )	log K <sub>ow</sub>	log BCF
<i>Hard</i>				
HCB	0.0062	3,500 - 10,000	5.3	3.5
DDT	0.0034	115	3.9 - 6.2	2.2 - 4.3
Toxaphene	n/a	85	2.9 - 3.3	1.2 - 1.6
Dieldrin	0.20	46	5.1 - 6.2	3.3 - 4.3
Mirex	0.20	700	5.8	3.9
<i>Soft</i>				
Malathion	145	1,375 - 2,800	2.7	1.0
Parathion	24	3.6 - 13	n/a	
Atrazine	30	1,870 - 3,080	2.3	0.7



**Figure 5-16.** Structure of 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (TCDD). The rings are numbered as shown.

## Dibenzofuran



**Figure 5-30.** Basic structure of dibenzofuran. Positions 1 through 4 and 6 through 9 have attached hydrogens that can be replaced by chlorines in chlorodibenzofurans.

**Table 5-10.** Toxicity equivalence factors (TEQ) for some important dioxins and furans

Dioxin or furan	TEQ
2,3,7,8-tetrachlorodibenzo- <i>p</i> -dioxin	1
1,2,3,7,8-pentachlorodibenzo- <i>p</i> -dioxin	0.5
1,2,3,4,7,8-hexachlorodibenzo- <i>p</i> -dioxin	0.1
1,2,3,7,8,9-hexachlorodibenzo- <i>p</i> -dioxin	0.1
1,2,3,6,7,8-hexachlorodibenzo- <i>p</i> -dioxin	0.1
1,2,3,4,6,7,8-heptachlorodibenzo- <i>p</i> -dioxin	0.01
octachlorodibenzo- <i>p</i> -dioxin	0.001
2,3,7,8-tetrachlorodibenzofuran	0.1
2,3,4,7,8-pentachlorodibenzofuran	0.5
1,2,3,7,8-pentachlorodibenzofuran	0.05
1,2,3,4,7,8-hexachlorodibenzofuran	0.1
1,2,3,7,8,9-hexachlorodibenzofuran	0.1
1,2,3,6,7,8-hexachlorodibenzofuran	0.1
2,3,4,6,7,8-hexachlorodibenzofuran	0.1
1,2,3,4,6,7,8-heptachlorodibenzofuran	0.01
1,2,3,4,7,8,9-heptachlorodibenzofuran	0.01
octachlorodibenzofuran	0.001

**Table 5-11. Solubility of BTEX aromatic hydrocarbons in water**

BTEX hydrocarbon	Solubility in distilled water (ppm)	Solubility in sea water (ppm)	Reference
Benzene	1696	201	1
Toluene	580	50	1
Ethylbenzene	161	111	2
<i>o</i> -xylene	171	130	2
<i>m</i> -xylene	148	106	2
<i>p</i> -xylene	156	111	2

**Table 5-12. Common DNAPLs**

Halogenated Volatiles	Nonhalogenated Semivolatiles
Chlorbenzene	2-Methyl naphthalene
1,2-Dichloropropane	<i>o</i> -Cresol
1,1-Dichloroethane	<i>p</i> -Cresol
1,1-Dichloroethylene	2,4-Dimethylphenol
1,2-Dichloroethane	<i>m</i> -Cresol
<i>trans</i> -1,2-Dichloroethylene	Phenol
<i>cis</i> -1,2-Dichloroethylene	Naphthalene
1,1,1-Trichloroethane	Benzo[ <i>a</i> ]anthracene
Methylene chloride	Fluorene
1,1,2-Trichloroethane	Acenaphthene
Trichloroethylene	Anthracene
Chloroform	Dibenzo[ <i>a,h</i> ]anthracene
Carbon tetrachloride	Fluoranthene
1,1,2,2-Tetrachloroethane	Pyrene
Tetrachloroethylene	Chrysene
Ethylene dibromide	2,4-Dinitrophenol
Halogenated Semivolatiles	Miscellaneous
1,4-Dichlorobenzene	Coal Tar
1,2-Dichlorobenzene	Creosote
Aroclor 1242, 1254, 1260	
Chlordane	
Dieldrin	
2,3,4,5-Tetrachlorophenol	
Pentachlorophenol	

**Figure 5-31.** Structures of some common organic acids and their dissociation constants,  $pK_a$ . Oxalic and sigma-phthalic acid have two dissociations constants because both acids have two-step dissociations. After Drever (1997).

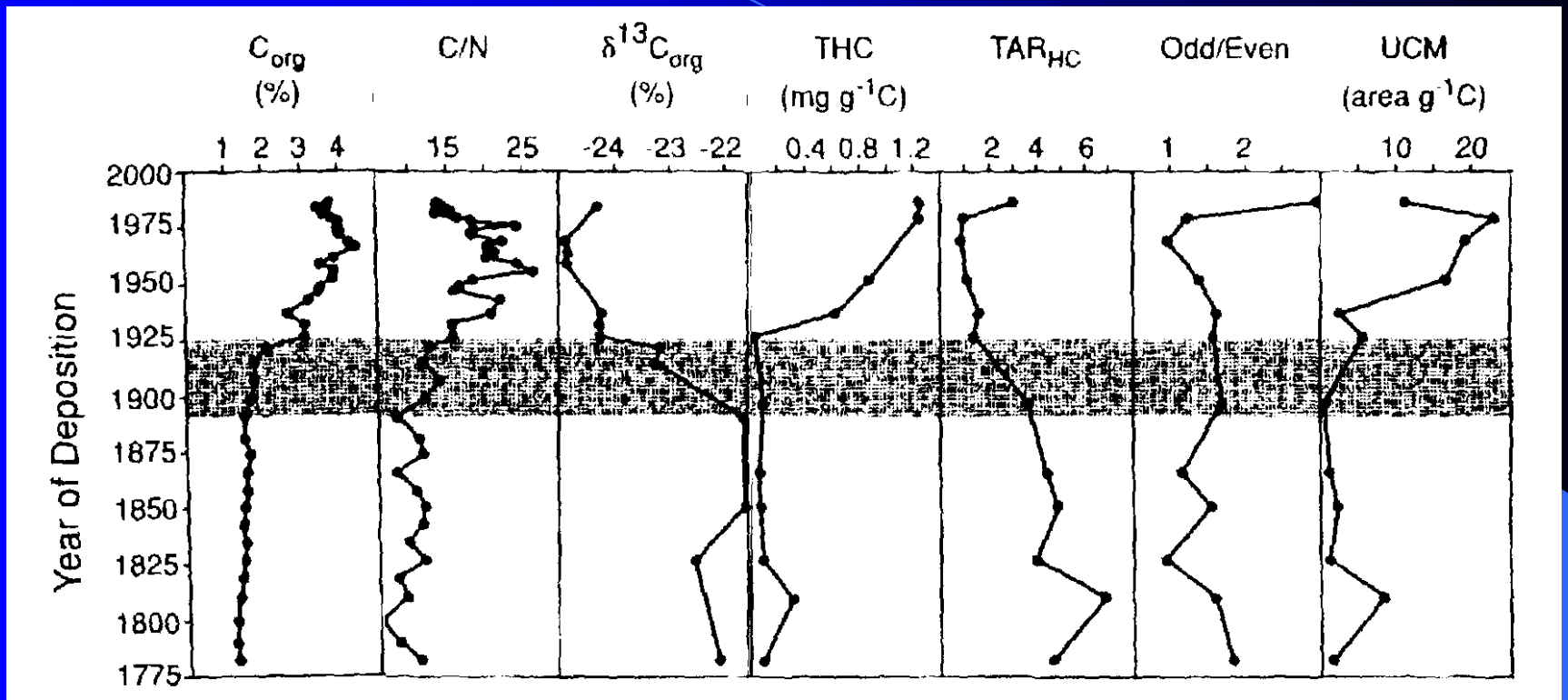
Acid	Structure	$pK_a$
Acetic	$CH_3COOH$	4.9
Lactic	$  \begin{array}{c}  CH_3-CH-COOH \\    \\  OH  \end{array}  $	3.1
Oxalic	$  \begin{array}{c}  COOH \\    \\  COOH  \end{array}  $	1.2, 4.2
Benzoic		4.2
$\sigma$ -Phthalic		2.9, 5.5

**Table 5-13.  $K_{oc}$  and Henry's Law constants for selected organic chemicals**

Compound	log $K_{oc}$	H (unitless)
DDT	5.18	0.00213
Hexachlorobutadiene	4.46	186.797
1,2-Dichlorobenzene	3.23	0.07889
Lindane	3.11	0.00333
Napthalene	3.11	0.04701
Ethylbenzene	3.04	0.26282
m-Xylene	2.99	0.43736
o-Xylene	2.92	0.20846
4-Chloro-m-cresol	2.69	0.00010
Tetrachloroethene	2.56	1.05865
Toluene	2.48	0.26037
Benzene	1.92	0.22849
2,4-D	1.78	7.7E-9
Dichlorodifluoromethane	1.76	121.39765
Bromobenzene	2.18	0.07848

**Table 5-14. Half-lives for selected organic chemicals**

Compound	Half-life in days			
	Aerobic decomposition		Anaerobic decomposition	
	Minimum	Maximum	Minimum	Maximum
Cresol(s)	<1	29	10	49
Phenol	<1	4	8	28
Napthalene	1	20	25	258
Toluene	4	22	56	210
Benzene	5	16	112	720
Xylene(s)	7	28	180	360
Methyl parathion	15	70	1	7
Aldecarb	20	361	62	635
Lindane	31	413	6	31
Dieldrin	175	1080	1	7
Tetrachloroethene	180	360	98	1653
Chlordane	238	1386	1	7
DDT	730	5708	16	100



**Figure 5-C3-1.** Organic carbon concentrations ( $C_{org}$ ), organic matter C/N ratios,  $\delta^{13}C_{org}$ , total extractable hydrocarbons (THC), concentration ratios of terrigenous/aquatic *n*-alkanes ( $TAR_{HC}$ ), odd/even *n*-alkanes and unresolved complex mixture (UCM) relative to sediment age. Shaded area represents time of greatest environmental change as determined from the sediment record. Modified from Tenzer et al. (1999).