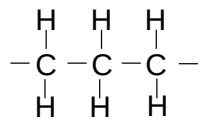
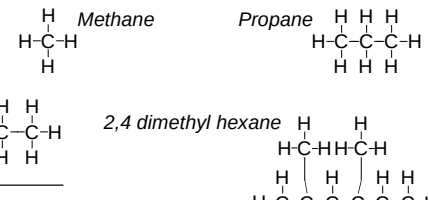
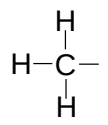
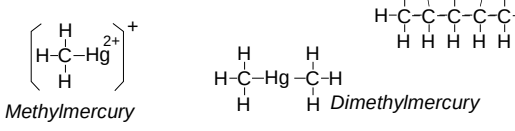
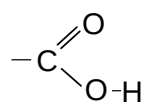
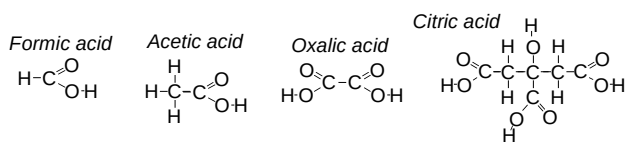
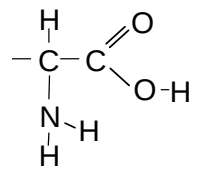
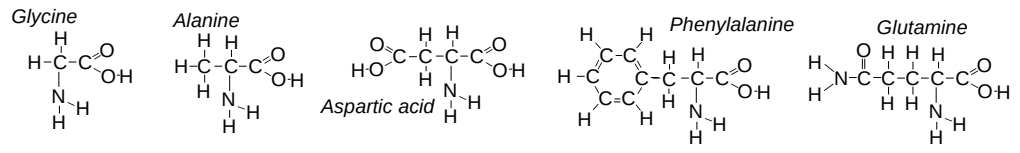
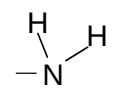
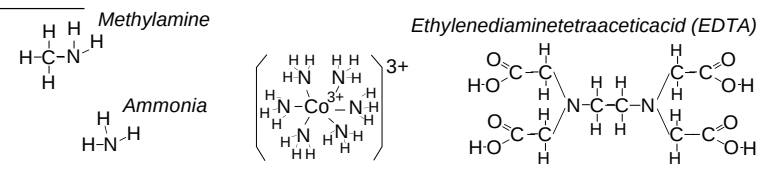
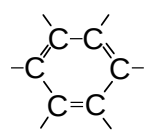
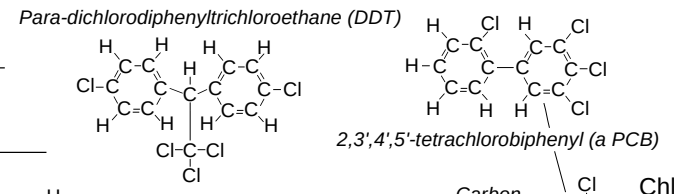
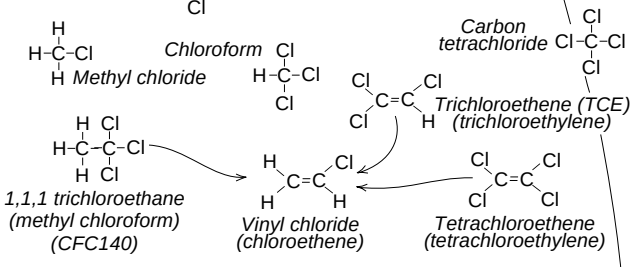
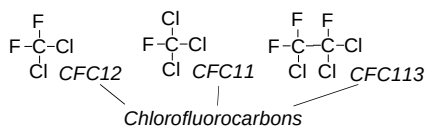
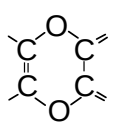
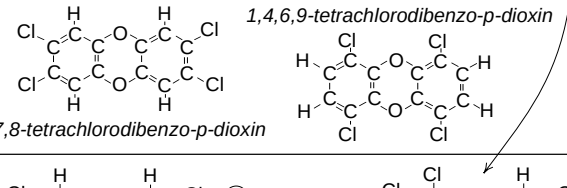
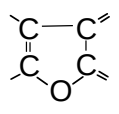
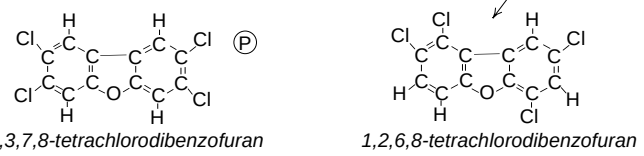
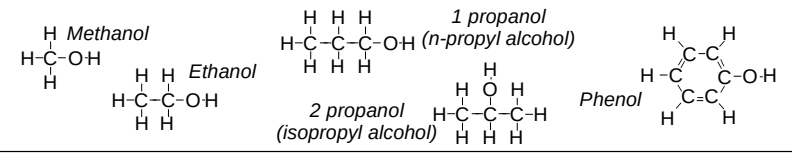
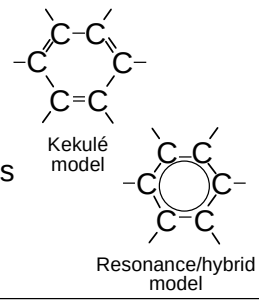
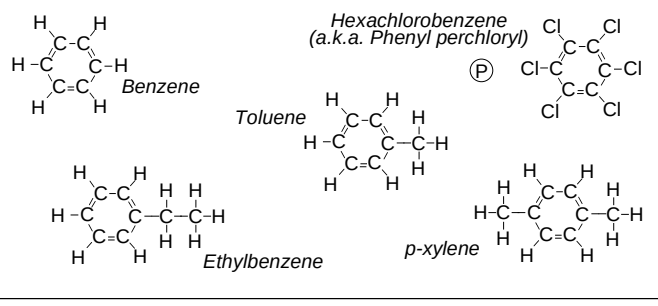
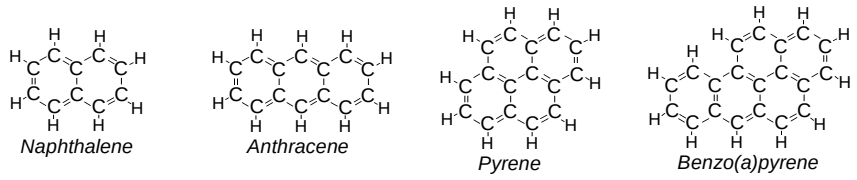
# Organic Structures and Functional Groups Relevant to Geochemistry and Environmental Chemistry

| Name | Structure | Examples* | Comments |
|---|---|---|---|
| Alkanes |  |   | Alkanes are chains of C atoms joined only by single bonds. Alkenes are chains in which at least two C atoms are joined by a double bond, and alkynes are chains in which at least two C atoms are joined by a triple bond.<br>Alkanes are a major component of petroleum, from methane in natural gas to longer chains in oils (both crude and refined). Longer chain length gives greater density (lesser API gravity), greater viscosity, and higher melting T. |
| Methyl groups |  |   | Methyl groups complex with cations, enhancing passage of the latter through cell membranes and thus into organisms. For example, methylmercury ($CH_3Hg^+$) is a toxin that bioaccumulates in food chains, causing Minimata disease. |
| Carboxyl groups |  |   | When undissociated, carboxyl groups are a source of $H^+$ ions. When dissociated, the single-bonded oxygen becomes a ligand atom for hard and intermediate cations. Solutes with carboxyl groups can thus be important in complexing (and thus in increasing the solubility of) many ions, especially $Al^{3+}$. Carboxyl groups are a major component of humic substances. |
| Amino acids |  |   | Amino acids contain a group consisting of a carboxyl group (see above) and an amine group (see below). There are twenty amino acids that are common in proteins. |
| Amines |  |   | Methane is surrounded by four evenly spaced $H^+$s (a tetrahedron of $H^+$s) and so has no polarity. In contrast, the N of ammonia and amines has only three $H^+$s in three of the same positions, leaving a fourth locus of negative charge. That fourth position makes N atoms strong ligands for hard to intermediate cations, so that ammonia has considerable dissolving power and amine-bearing compounds are effective complexers. |
| Phenyl groups |  |   | A phenyl group is a benzene molecule (see below) with at least one H replaced with some other group. Many noteworthy pollutants contain phenyl groups, such as PCBs (polychlorinated biphenyls (left)), dioxins and furans (below), and hexachlorobenzene (HCB, farther below). PCBs are among the Persistent Organic Pollutants (Ⓟ). |
| Chloride −Cl | |   | Chlorinated organic compounds are among the most noteworthy toxic and persistent pollutants. These include hexachlorobenzene (below), DDT and PCBs (at left), and dioxins and furans (below). Trichloroethylene (TCE) is used as an industrial solvent, is found in about one third of US groundwater supplies, and is the most common pollutant detected at Superfund sites. Tetrachloroethylene is a solvent used in dry cleaning and is thus a wide-spread pollutant. Trichloroethylene, tetrachloroethylene, and trichloroethane are transformed to vinyl chloride, a toxic carcinogen. Chloroform is a suspected carcinogen that forms as a byproduct of chlorination of drinking water. |
| Fluoride −F | |   | The chlorofluorocarbons CFC11 and CFC12 were used as refrigerants and propellants, CFC113 and methyl chloroform were used as industrial solvents, and CFC12 was used to make the bubbles in styrofoam. All catalyze destruction of ozone in the upper atmosphere and have lifetimes of several decades there. To get from a CFC code to a chemical formula, add 90 to the code. In the result, the first number is the number of C atoms, the second the number of H atoms, and the third is the number of F atoms; the number of Cl atoms is deduced as the remainder. |
| Dioxins Ⓟ |  |   | Of the many dioxin compounds, the 2,3,7,8 tetrachlorodibenzo-p-dioxin molecule shown here is the most toxic and so is the one known colloquially as "dioxin". The 1,4,6,9 molecule, on the other hand, is seemingly the least toxic. |
| Furans Ⓟ |  |   | Dibenzofurans form when PCBs are heated and an oxygen bridges between the two phenyl groups. |
| Alcohols −O−H | |   | Ethyl alcohol (ethanol) is the excrement of yeast found in beer, wine, and liquor. It is produced from sugar cane, corn, and other plant material. Methyl alcohol (methanol) is toxic, causing blindness and death in small quantities. It is produced from fossil hydrocarbons. Methanol's high solubility makes it difficult to separate from water. Spills of the toxin into drainage systems or other waters are thus especially problematic. |
| Aromatic compounds |   |   | Aromatic compounds are those with a Kekulé structure, a six-fold ring of C atoms in which each C is bonded to one atom outside the ring. The ring is commonly portrayed as having three single bonds and three double bonds between the C atoms, but it is better envisioned a resonance hybrid bond.<br>Benzene, toluene, and xylene are present in gasoline and collectively called the BTX component. The BTX component is the most toxic part of petroleum. Benzene, toulene, and ethylbenzene are, with TCE, the most common organic pollutants at Superfund sites. |
| Polycyclic Aromatic Hydrocarbons (PAHs) | |   | Polycyclic (or polynuclear) aromatic hydrocarbons form via the incomplete combustion of organic matter and fossil fuels (from coal soot to the black on grilled foods). PAHs are thus air pollutants and water pollutants. Several are carcinogens, of which benzo(a)pyrene is the most potent. Graphite is the PAH of effectively infinite linkage. |

Ⓟ The United Nations Environmental Programme (UNEP) has recognized 12 chemicals or classes of chemicals as Persistent Organic Pollutants (POPs). All twelve are Cl-bearing chemicals with at least one ring of five carbons or six carbons.

*Some examples serve for two rows (for example, 2,4 dimethyl hexane is an example of an alkane and of a structure with methyl groups).


Sources: Baird, C., 1995, *Environmental Chemistry:* New York, W.H. Freeman and Company, 484 p.
Hart, H., *Organic Chemistry* (8th edn.): Boston, Houghton Mifflin Company, 537 p.
Schwarzenbach, R.P., Gschwend, P.M., & Imboden, D.M., 2003, *Environmental Organic Chemistry:* Hoboken, Wiley-Interscience, 1313 p.
United Nations Environment Program, *Persistent Organic Pollutants:* http://www.chem.un.ch/pops/



Acknowledgments:
This table was greatly improved by the comments of Dr. Valentine Nzengung. "Fungal Excrement" (and hence "excrement of yeast") is a phrase used by Dr. Charles Mims.



Citation: Railsback, L. Bruce, 2004, Organic Structures and Functional Groups Relevant to Geochemistry and Environmental Chemistry (unpublished).