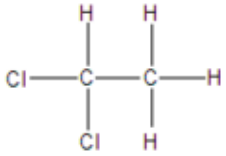
Naming alkanes with halogens

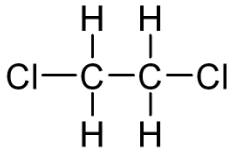
In naming a molecule which contain halogens (F,Cl,Br, and I) we treat the halogen just like an alkyl group and indicate its presence with the following names:

fluoro	for	F
chloro	for	C1
bromo	for	Br
iodo	for	I

Older common names for simple halogenated compounds often use the ionic form of the halogen name i.e. fluoride, chloride, bromide, and iodide even though no ionic bond is present.
CH_3Cl is named chloromethane. The older name is methyl chloride.
CH_3Br is named bromomethane. The older name is methyl bromide
.
Let's look at some examples:
a)Two molecules with which we introduced the concept of structural isomers:



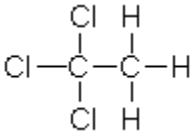
1,1-dichloroethane



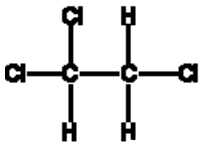
1,2-dichloroethane

The longest carbon chain in both cases is ethane and in both cases there are two chlorine atoms so name them both dichloroethane. However in the first case both C1 atoms are on the same C atom so call it 1,1-dichloroethane. In the second molecule the C1 atoms are on different carbon atoms so we indicate that as 1,2-dichloroethane.

b)Two isomers with the formula $C_2H_3C1_3$

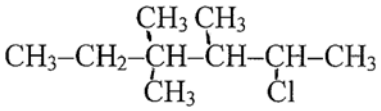


1,1,1-trichloroethane
(not 2,2,2-trichloroethane
and not 1-trichloroethane)



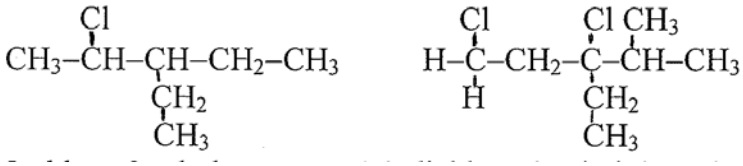
1,1,2-trichloroethane
(not 1,2,2-trichloroethane)

c) A molecule with both alkyl and halogen groups



Numbering from left to right: 5-chloro-3,3,4 trimethylhexane Sum of numbers is 15
Numbering from right to left: 2-chloro-3,4,4-trimethylhexane Sum of number is 13.
Numbering from right to left gives the correct name.

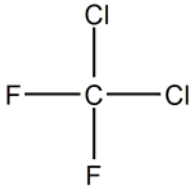
d)

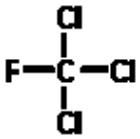


2-chloro-3-ethylpentane 1,3-dichloro-3-ethyl-4-methylpentane
What would the numbering be if we numbered from right to left?

Examples with practical uses:

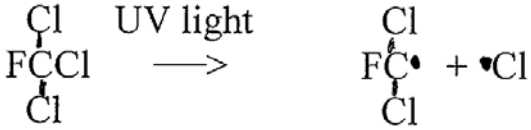
Freons





Dichlorodifluoromethane (Freon12) chlorotrifluoromethane (Freon13) trichlorofluoromethane (Freon 11)

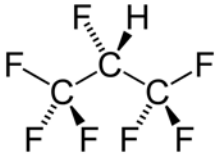
Freon 12 and other Freons have been used as the gases in refrigerators and air conditioners, but when they escape to the upper atmosphere, UV radiation can break the C-Cl bond and produce Cl free radicals (molecules with unpaired electrons) which can then destroy ozone in the upper atmosphere.



Chlorofluorocarbons(CFC's) were phased out in developed countries for spray cans in 1978, for refrigerators and air conditioners in 1995, and for medical inhalers (**metered dose inhalers** or MDI's for inhaled drugs such as **albuterol**) as of 2008. They have been replaced with hydrofluoroalkanes (HFAs) 134a and 227 which are *less* damaging to the ozone layer. (The hydrofluoroalkanes are less damaging to the ozone layer because the C-F bond is not as susceptible breakage by UV radiation as the C-Cl bond.)

HFA 134a has the structure
and the systematic name 1,1,1,2-tetrafluoroethane

HFA 227 has the wedge and dash structure

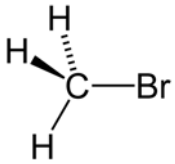


and the systematic name 1,1,1,2,3,3,3-heptafluoropropane.

Notice that both of these molecules contain only F halogen atoms and no Cl atoms. The C-F bond is much more resistant to UV light than the C-Cl bond. The substitution of HFAs for CFCs is more complicated than you might think and has required extensive research in the last two decades. The HFAs are more expensive to produce and large scale testing of efficacy and toxicity of the newly reformulated inhalers was required by the FDA. The cost of metered dose inhalers (MDIs) using HFAs are substantially more expensive than the old inhalers using CFCs.

Two albuterol inhalers reformulated with HFAs.

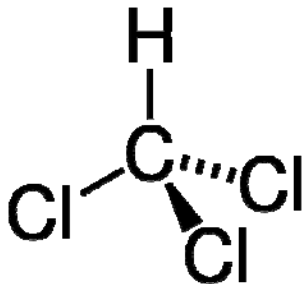
Bromomethane (Methyl bromide)



IUPAC: bromomethane
Common: methylbromide

Bromomethane (methyl bromide) has been used as a specialized soil fumigant, especially for growing strawberries. It is extremely toxic and great care must be taken in applying it. Methyl bromide is also a very potent ozone destroyer and there have been calls for taking it off the market for many years.

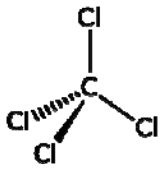
Trichloromethane(chloroform)



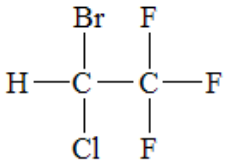
Trichloromethane (chloroform) was one of the earliest general anesthetics (a molecule which induces sleep as well as analgesia). It was administered by breathing the vapors of liquid chloroform and was first used during childbirth in 1847. It competed strongly with ether for the next 60 years as the general surgical anesthetic of choice. It has a sweet smell and is much less flammable and less irritating than ether, but the risk of putting the patient to sleep permanently is higher than for ether. Lethal overdose with chloroform was all too frequent and it could cause cardiac arrhythmias. Accumulated data published in 1934 showed that deaths from chloroform anesthesia were over four times as frequent as those with ether anesthesia (about 1 in 3000 for chloroform vs 1 in 14,000 for ether anesthesia). It is no longer use as an anesthetic.

It continued to be used in some cough suppressants and toothpastes and other cosmetics until such use was banned in 1976 based on data from rats that it could cause birth defects and liver cancer. Current exposure in the US is very small, primarily from chlorinated water reacting with organic compounds in the water to form trace amounts of chloroform in drinking water.

Tetrachloromethane(carbon tetrachloride)



Tetrachloromethane(carbon tetrachloride**) w**as commonly used as a drycleaning solvent in the first half of the twentieth century to remove grease and dirty from clothes.. It was also used in the synthesis of the Freon gases for refrigerators and air conditioners. Exposure to CCl_4 was associated with neurological, liver, and kidney damage and it was replaced as a dry cleaning solvent. Like the Freon molecules, CCl_4 can cause ozone depletion and its use has dropped dramatically.

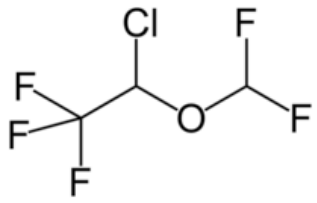


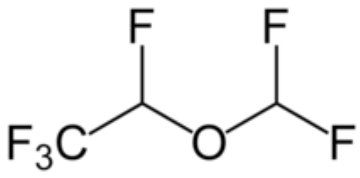
IUPAC: 2-bromo-2-chloro 1,1,1-trifluoroethane
Common: halothane

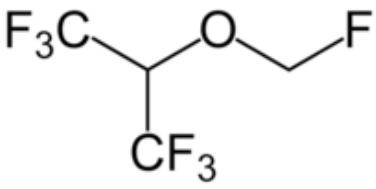
This molecule has the common name of **halothane**(suggest why!). It came on the market n 1956 and replaced ether as the anesthetic of choice because it was less irritating to the airway and it was not flammable. It did however have some adverse effects including cardiac depression (slowing of the heart rate) and rare (1 in 35,000) cases of hepatitis. It gradually lost "market share" to safer anesthetics.

Current inhalation anesthetics:

The current most commonly used inhalation anesthetics are halogenated ethers shown below which eliminate the flammability problem of ether and are generally less irritating to the airway than ether.





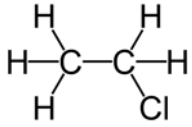


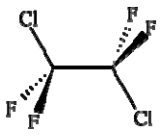
Isoflurane **Desflurane** **Sevoflurane**

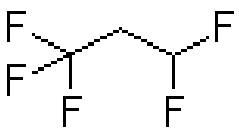
The mechanism of action of general anesthetics is poorly understood, is very complex, and probably involves many different factors. They appear to inhibit movement of the action potential along neurons as well as activating or inactivating a wide variety of neuronal receptors.

Topical anesthetics that work by chilling the skin surface

Name the following three molecules:

a)


b)


c)


1 chloroethane
ethyl chloride

1,2-dichloro-1,1,2,2-tetrafluoroethane

1,1,1,3,3-pentafluoropropane

a)The first molecule has the common name ethyl chloride and has been used as a mild topical anesthetic while doing minor surgeries (e.g. removing a deep splinter). It has a low boiling point (12 ^{o}C) and boils off the skin (at 37^{o}C), lowering the skin temperature in the process and decreasing pain sensation. It is occasionally used as a recreational inhalant. Its use is decreasing..
b)The second molecule, 1,2-dichloro-1,1,2,2-tetrafluroethane, is marketed under the trade name, Frigiderm, works by a similar mechanism. It has a boiling point of 4^{o}C.

c) The third molecule, 1,1,1,3,3-pentafluoropropane, is marketed under the name Gebauer's Spray and Stretch. It is marketed for reducing pain of sprains. (Boiling point = 14^{o}C)


Perfluoroalkanes (completely fluorinated C chains) are liquids which dissolve large amounts of oxygen while remaining biologically inert. Such fluids were the basis for the oxygenated liquid in the movie The Abyss. Perfluoroalkanes have been investigated for filling the lungs of premature infants with respiratory distress syndrome. Clinical trials of one such liquid (Liquivent) were disappointing and it was not approved for market. Perfluorochemicals are also accumulating in the environment due to their invertness, albeit in small concentrations. They can accumulate in the fat of animals (including humans). Although their short-term toxicity appears to be low, long term data is minimal and there is increasing concern about the long term biological effects of perfluorochemicals accumulating in the body.

Perfluorochemicals have also been investigated for their use as artificial blood which could be used instead of real blood for blood transfusions. Perfluorochemicals would have the advantage of not having to match blood types and would not require testing for viral contamination with HIV and hepatitis which are necessary for blood transfusions. More recent research has been done on an emulsion of perfluorochemical, water, and lecithin) with the trade name Oxygent ^{TM}. There is definitely a demand for a blood substitute, but that product has not yet been widely marketed.