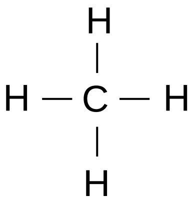
Hydrocarbon Fuels (quick overview)

Most common hydrocarbon fuels are **Alkyl Compounds** and are grouped as:

Paraffins (alkanes): single-bonded, open-chain, saturated

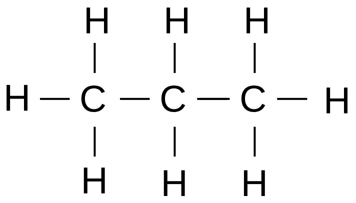
C_nH_{2n+2}

n= 1 CH_4 methane
n= 2 C_2H_6 ethane
n= 3 C_3H_8 propane
n= 4 C_4H_{10} butane
n= 8 C_8H_{18} n-octane and isooctane



$$\begin{array}{ccccc} & & H & & \\ & & | & & \\ H & - & C & - & H \\ & & | & & \\ & & H & & \end{array}$$

methane



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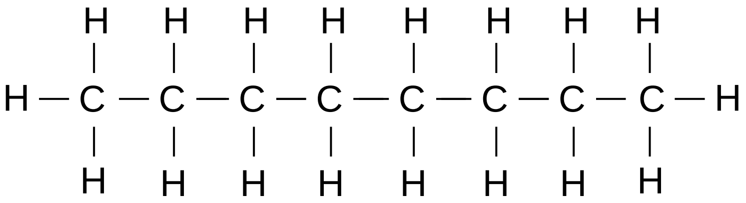
propane



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n-octane

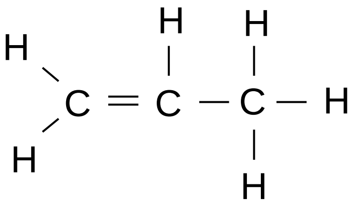
There are multiple isooctanes, depending on position of methyl (CH_3) branches which replace hydrogen atoms (eg. 3 H are replaced with 3 CH_3)

Hydrocarbon Fuels (cont'd)

Olefins (alkenes): open-chain containing one double-bond, unsaturated (break bond more hydrogen can be added)

C_nH_{2n}

n=2 C_2H_4 ethene
n=3 C_3H_6 propene



propene

Acetylenes (alkynes): open-chain containing one C-C triple-bond unsaturated

C_nH_{2n-2}

n=2 C_2H_2 acetylene
n=3 C_3H_4 propyne

$H-C\equiv C-H$

acetylene

For **alcohols** one hydroxyl (OH) group is substituted for one hydrogen
e.g. methane becomes methyl alcohol (CH_3OH) or **methanol**
ethane becomes ethyl alcohol (C_2H_5OH) or **ethanol**

Atom Balancing

If sufficient oxygen is available, a hydrocarbon fuel can be completely oxidized, the carbon is converted to carbon dioxide (CO_2) and the hydrogen is converted to water (H_2O).

The overall chemical equation for the complete combustion of one mole of propane (C_3H_8) is:

$$C_3H_8 + aO_2 \rightarrow bCO_2 + \underset{\overset{\uparrow}{\text{\# of moles}}}{c}\,\underset{\overset{\uparrow}{\text{species}}}{H_2O}$$

Elements can not be created or destroyed so

carbon balance gives $b = 3$

hydrogen balance gives $2c = 8 \rightarrow c = 4$

oxygen balance gives $2b + c = 2a \rightarrow a = 5$

Thus the above reaction is:

$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$$

Generalized Atom Balancing

Air contains molecular nitrogen N_2, when the products are low temperature the nitrogen is not significantly affected by the reaction, it is considered **inert**.

The complete reaction of a general hydrocarbon $C_\alpha H_\beta$ with air is:

$$C_\alpha H_\beta + \left(\alpha + \frac{\beta}{4}\right)(O_2 + 3.76N_2) \rightarrow \alpha CO_2 + \frac{\beta}{2}H_2O + 3.76\left(\alpha + \frac{\beta}{4}\right)N_2$$

The above equation defines the **stoichiometric** proportions of fuel and air.

Example: For propane (C_3H_8) α= 3 and β= 8

$$C_3H_8 + (5)(O_2 + 3.76N_2) \rightarrow 3CO_2 + 4H_2O + 3.76(5)N_2$$

Generalized A/F Ratio Determination

The air/fuel and fuel/air ratio on a mass basis is:

$$(A/F)_s = \frac{1}{(F/A)_s} = \frac{\left(\alpha + \frac{\beta}{4}\right)\overline{M}_{O_2} + 3.76\left(\alpha + \frac{\beta}{4}\right)\overline{M}_{N_2}}{\alpha\overline{M}_C + \beta\overline{M}_H}$$

Substituting the respective molecular weights and dividing top and bottom by α one gets the following expression that only depends on the ratio of the number of hydrogen atoms to hydrogen atoms *(β/α)* in the fuel.

$$(A/F)_s = \frac{1}{(F/A)_s} = \frac{\left(1 + \frac{(\beta/\alpha)}{4}\right)(32 + 3.76 \cdot 28)}{12 + (\beta/\alpha) \cdot 1}$$

Note above equation only applies to **stoichiometric mixtures**

For methane (CH_4), $\beta/\alpha = 4$ → $(A/F)_s = 17.2$

For propane (C_3H_8), $\beta/\alpha = 2.67$ → $(A/F)_s = 15.6$