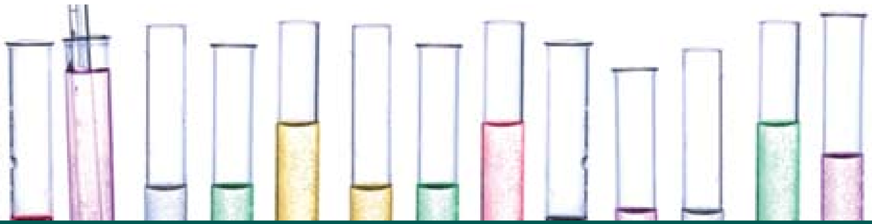

Set 29: Calculations Involving Hydrocarbons

1. $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

   $M(CH_4) = 16.042 \text{ g mol}^{-1}$

   $$n(CH_4) = \frac{m}{M} = \frac{31\times10^3}{16.042} = 1935.427 \text{ mol}$$

   $n(CO_2) = n(CH_4) = 1932.427 \text{ mol}$
   $M(CO_2) = 44.01 \text{ g mol}^{-1}$
   $m(CO_2) = nM = 1932.427 \times 44.01 = 85046.13 \text{ g} = 85 \text{ kg}$

2. $C_3H_8 + 10O_2 \rightarrow 6CO_2 + 8H_2O$
   $M(C_3H_8) = 44.094 \text{ g mol}^{-1}$

   $$n(C_3H_8) = \frac{m}{M} = \frac{34.0\times10^3}{44.094} = 771.0799 \text{ mol}$$

   $n(CO_2) = {}^6/_2 n(C_3H_8) = {}^6/_2(771.0799) = 2313.2398 \text{ mol}$
   $M(CO_2) = 44.01 \text{ g mol}^{-1}$
   $m(CO_2) = nM = 2313.2398 \times 44.01 = 101805.7 \text{ g} = 102 \text{ kg}$

3. Methane is fluorinated in two steps. In each step one hydrogen atom is replaced by a fluorine atom. The overall equation to represent the process is

   $CH_4 + 2F_2 \rightarrow CH_2F_2 + 2HF$
   $M(CH_2F_2) = 52.026 \text{ g mol}^{-1}$

   $$n(CH_2F_2) = \frac{m}{M} = \frac{8.00\times10^3}{52.026} = 153.769 \text{ mol}$$

   $n(CH_4) = n(CH_2F_2) = 153.769 \text{ mol}$
   $M(CH_4) = 16.042 \text{ g mol}^{-1}$
   $m(CH_4) = nM = 153.769 \times 16.042 = 2466.8 \text{ g} = 2.47 \text{ kg}$

4. (a) $CH_4 + F_2 \rightarrow CH_3F + HF$

$CH_3F + F_2 \rightarrow CH_2F_2 + HF$

$CH_2F_2 + F_2 \rightarrow CHF_3 + HF$

Overall: $CH_4 + 3F_2 \rightarrow CHF_3 + 3HF$

(b) $M(CHF_3) = 70.018\ g\ mol^{-1}$

$$n(CHF_3) = \frac{m}{M} = \frac{2.50\times10^3}{70.018} = 35.7051\ mol$$

$n(CH_4) = n(CHF_3) = 35.7051\ mol$

$M(CH_4) = 16.042\ g\ mol^{-1}$

$m(CH_4) = nM = 35.7051 \times 16.042 = 572.78\ g = 0.573\ kg$

5. (a) An addition reaction can be used. Specifically hydrogenation would add two hydrogen atoms to each double bond in the hydrocarbon chain.
Reagents required are hydrogen gas and a metal catalyst such as nickel, platinum or palladium.

(b) Each molecule has three double bonds converted to single bonds. The reaction can be represented as follows

$C_{57}H_{102}O_6 + 3H_3 \rightarrow C_{57}H_{108}O_6$

$M(C_{57}H_{102}O_6) = 883.386\ g\ mol^{-1}$

$$n(C_{57}H_{102}O_6) = \frac{m}{M} = \frac{450}{883.386} = 0.5094\ mol$$

$n(H_2) = 3n(C_{57}H_{102}O_6) = 3 \times 0.5094 = 1.5282\ mol$

$M(H_2) = 2.016\ g\ mol^{-1}$

$m(H_2) = nM = 1.5282 \times 2.016 = 3.08\ g$

6. (a) Methane is fluorinated in two steps. In each step one hydrogen atom is replaced by a fluorine atom. The overall equation to represent the process is

$CH_4 + 2F_2 \rightarrow CH_2F_2 + 2HF$

$m(CH_2F_2) = 50\%\ of\ 1.00\ kg = 500\ g$

$M(CH_2F_2) = 52.026\ g\ mol^{-1}$

$$n(CH_2F_2) = \frac{m}{M} = \frac{500}{52.026} = 9.611\ mol$$

$n(CH_4) = n(CH_2F_2) = 9.611\ mol$

$M(CH_4) = 16.042\ g\ mol^{-1}$

$m(CH_4) = nM = 9.611 \times 16.042 = 154\ g$

(b) Pentafluoroethane can be produced by a combination of addition reactions (two) and a substitution reaction from the starting material ethyne.
Note: There are other , but more difficult, pathways to produce pentafluoroethane from ethyne.

$C_2H_2 + F_2 \rightarrow CHFCHF$

$CHFCHF + F_2 \rightarrow CHF_2CHF_2$

$CHF_2CHF_2 + F_2 \rightarrow CHF_2CF_3 + HF$

Overall: $C_2H_2 + 3F_2 \rightarrow CHF_2CF_3 + HF$

$m(CHF_2CF_3) = 50\%\ of\ 1.00\ kg = 500\ g$

$M(CHF_2CF_3) = 120.028\ g\ mol^{-1}$

$$n(CHF_2CF_3) = \frac{m}{M} = \frac{500}{120.028} = 4.1657\ mol$$

$n(C_2H_2) = n(CHF_2CF_3) = 4.1657\ mol$

$M(C_2H_2) = 26.036\ g\ mol^{-1}$

$m(C_2H_2) = nM = 4.1657 \times 26.036 = 108\ g$

(c) Fluorine is required for all reactions to produce CH_2F_2 and CHF_2CF_3.

(d) From the overall equations

$n(F_2) = 3n(CHF_2CF_3) + 2n(CH_2F_2) = 3(4.1657) + 2(9.611) = 31.719\ mol$

$M(F_2) = 38.00\ g\ mol^{-1}$

$m(F_2) = nM = 31.719 \times 38.00 = 1205\ g = 1.21\ kg$

7. (a) $C_3H_8 + 10O_2 \rightarrow 6CO_2 + 8H_2O$

$M(C_3H_8) = 44.094\ g\ mol^{-1}$

$$n(C_3H_8) = \frac{m}{M} = \frac{0.500}{44.094} = 1.1339 \times 10^{-2}\ mol$$

$m(O_2) = 0.20 \times 10.0 = 2.00\ g$

$M(O_2) = 32.00\ g\ mol^{-1}$

$$n(O_2) = \frac{m}{M} = \frac{2.00}{32.00} = 6.25 \times 10^{-2}\ mol$$

$n(O_2)_{\text{required to use all the propane}} = {}^{10}/_{2}n(C_3H_8) = {}^{10}/_{2}(1.1339 \times 10^{-2}) = 5.6695 \times 10^{-2}\ mol$

There is therefore enough oxygen to use all the propane, so propane is the limiting reagent. Using the limiting reagent

$n(CO_2) = {}^{6}/_{2}n(C_3H_8) = {}^{6}/_{2}(1.1339 \times 10^{-2}) = 3.4017 \times 10^{-2}\ mol$

$M(CO_2) = 44.01\ g\ mol^{-1}$

$m(CO_2) = nM = 3.4017 \times 10^{-2} \times 44.01 = 1.497\ g = 1.50\ g$

(b) The reagent in excess is oxygen.

$n(O_2)_{\text{in excess}} = n(O_2)_{\text{initial}} - n(O_2)_{\text{reacted}} = 6.25 \times 10^{-2} - 5.6695 \times 10^{-2} = 5.805 \times 10^{-3}\ mol$

$m(O_2) = nM = 5.805 \times 10^{-3} \times 32.00 = 0.186\ g$

8. (a) $CH_4 + C\ell_2 \rightarrow CH_3C\ell + HC\ell$

$CH_3C\ell + C\ell_2 \rightarrow CH_2C\ell_2 + HC\ell$

Overall: $CH_4 + 2C\ell_2 \rightarrow CH_2C\ell_2 + 2HC\ell$

(b) $CH_3C\ell$, $CHC\ell_3$ and $CC\ell_4$

(c) Fractional distillation as boiling points of each compound is different as show in the table.

Compound	Boiling Point (°C)
$CH_3C\ell$	–24.0
$CH_2C\ell_2$	39.8
$CHC\ell_3$	62.0
$CC\ell_4$	76.8

(d) m(CH_4) = 22.5% of 1.00 kg = 225 g
M(CH_4) = 16.042 g mol^{-1}

$$n(CH_4) = \frac{m}{M} = \frac{225}{16.042} = 14.026 \text{ mol}$$

n($C\ell_2$) = 2n(CH_4) = 2 × 14.026 = 28.051 mol
M($C\ell_2$) = 70.90 g mol^{-1}
m($C\ell_2$) = nM = 28.051 × 70.90 = 1988.8 g = 1.99 kg

9. $2C_8H_{18} + 25O_2 \rightarrow 16CO_2 + 18H_2O$
m(C_8H_{18}) = 60.0 × 0.703 = 42.18 kg
M(C_8H_{18}) = 114.224 g mol^{-1}

$$n(C_8H_{18}) = \frac{m}{M} = \frac{42.18 \times 10^3}{114.224} = 369.274 \text{ mol}$$

n(CO_2) = $^{16}/_2$n(C_8H_{18}) = $^{16}/_2$(369.274) = 2954.192 mol
M(CO_2) = 44.01 g mol^{-1}
m(CO_2) = nM = 2954.192 × 44.01 = 1.30×10^5 g = 130 kg

10. (a) The overall reaction is $CH_4 + 4Br_2 \rightarrow CBr_4 + 4HBr$
M(CBr_4) = 331.61 g mol^{-1}

$$n(CBr_4) = \frac{m}{M} = \frac{136}{331.61} = 0.410 \text{ mol}$$

n(CH_4) = n(CBr_4) = 0.410 mol
M(CH_4) = 16.042 g mol^{-1}
m(CH_4) = nM = 0.410 × 16.042 = 6.58 g

(b) n(Br_2) = 4n(CBr_4) = 4 × 0.410 = 1.64 mol
M(Br_2) = 159.8 g mol^{-1}
m(Br_2) = nM = 1.64 × 159.8 = 262 g

(c) The limiting reagent is bromine as there none left in the reaction mixture.
Some bromine will have ended up in other bromomethanes. It is likely that some CH_3Br, CH_2Br_2 and $CHBr_3$ is present in the reaction mixture.