Air Pollution
ENV-409
Emissions and Control Solutions

The table provided gives bond energies as positive values. Energy is released from the formation of a bond, so they should be negative according to the convention of standard heats of formation ($\Delta_f H^0$ is negative for exothermic reactions). The positive values indicate the same magnitude of energy needed to break a bond ("bond dissociation energy") so we calculate the heat of combustion from "products minus reactants" and use the provided ΔH^0's with opposite sign (as negative values instead of positive ones).

Hint for shortcut

Recall that

$$C_xH_y + \left(x + \frac{y}{4}\right) O_2 \rightarrow xCO_2 + \frac{y}{2}H_2O$$

Saturated alkanes with carbon number of x can be represented as $CH_3(CH_2)_{(x-2)}CH_3$ or $H(CH_2)_xH$. So y can be written as a function of x. Also, you will need to consider the breaking of C−C bonds. The number of these bonds can also be written as a function of x.

Solution

$y = 2x + 2$ and the number of C−C is $x - 1$. So

$$C_xH_{2x+2} + \left(\frac{3x+1}{2}\right) O_2 \rightarrow xCO_2 + (x+1)H_2O$$

and

$$\Delta_c H^0(x) = \left[2x\Delta H^0_{\text{C=O}} + 2(x+1)\Delta H^0_{\text{O-H}}\right] - \left[(2x+2)\Delta H^0_{\text{C-H}} + \left(\frac{3x+1}{2}\right)\Delta H^0_{\text{O=O}} + (x-1)\Delta H^0_{\text{C−C}}\right]$$

The mass of carbon emitted per unit of heat is

$$\frac{x}{|\Delta_c H^0(x)|} \cdot \frac{44.01 \text{ g } CO_2/\text{mol}}{4.184 \text{ kJ/kcal}}$$

Example code in R:

```
DHc <- function(x) {
  reac. <- -c("C-H"=98.7,"C-C"=82.6,"O=O"=118.9) # reactants
  prod. <- -c(CO2=2*192,H2O=2*110.6)             # products
  y <- 2*x+2
  prod.%*%c(x,y/2)-reac.%*%c(y,x-1,x+y/4)
}
x <- c(1,8,14)
values <- x/abs(sapply(x,DHc))*44.01/4.184
```

Values:

compound	g CO_2/kJ
CH_4	0.054
C_8H_{18}	0.069
$C_{14}H_{30}$	0.07

According to this analysis, methane is the cleanest with respect to CO_2 emissions as it emits the least amount of CO_2 of these three fuels on an energy basis. It is indeed true that the case for using natural gas in the real world is (partially) made on the basis that its CO_2 emissions are smaller than other fossil fuels for the same amount of energy produced from combustion.