We can use Hess's Law (in combination with many other useful relationships we have learned this term) to tell us some interesting things about stable compounds with high potential energies (fuels).

Consider the following fuels (or potential fuels). Each group will be assigned three (and there will be some overlap to ensure we get the correct answers.

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| **Fuel** | **ΔH°f (kJ/mol)** | **density (g/L)** |
| *Hydrogen (H2)* | **0 (gas)** | **0.0899** |
| *Coal (C)* | **0 (solid)** | **1100** |
| *Natural Gas (methane, CH4)* | **–74.9 (gas)** | **0.667** |
| *Methanol (CH4O)* | **–238.4 (liquid)** | **791** |
| *Formaldehyde (CH2O)* | **–177.6 (solid)** | **880** |
| *Formic acid (CH2O2)* | **–425.0 (liquid)** | **1220** |
| *Propane (C3H8)* | **–103.8 (gas)**  **–104.7 (liquid)** | **1.88 (gas)**  **582 (liquid)** |
| *Octane (C8H18)* | **–208.4 (liquid)** | **703** |

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| --- | --- |
| **Compounds involved in combustion** | |
| *Oxygen (O2 (g))* | **ΔH°f = 0 kJ/mol** |
| *Carbon Dioxide (CO2 (g))* | **ΔH°f = –393.5 kJ/mol** |
| *Water (H2O (l))* | **ΔH°f = –285.8 kJ/mol** |

1) Begin by writing balanced combustion reactions for each of your assigned fuels. Combustion is the process where a fuel is reacted with oxygen (O2) to give carbon dioxide and/or water.

2) Use standard enthalpies of formation (provided below for all relevant species) to determine the enthalpy change associated with combustion of all three of your fuels (i.e., ΔH°rxn for the balanced combustion equations you wrote in part (1)).

3) Now let's calculate the energy density of your 3 fuels. We can define energy density in 3 related ways:

1. kJ of heat per mole of fuel
2. kJ of heat per gram of fuel
3. MJ of heat per liter of fuel (remember a megajoule is 106 J)

For each of your three assigned fuels, determine the energy content in each of the 3 above ways. Fill in your answers on the next sheet of this handout and, once you have solved for all 9 data points, enter your answers into the computer at the front of the classroom.

4) Due to concerns about global climate change, we are also very interested in CO2 emissions. For each of your three fuels, determine how many mmol of CO2 are produced per kJ of heat. Which is best?

5) Can you pick out any trends with respect to the different fuels? What elemental compositions are good? Which ones are not so good?

Why do some fuels perform better in some categories than others? How might this influence application?

What is our best bet if we want to minimize CO2? What are potential problems associated with this/these fuels?

6) We can use energy density as a metric for comparing chemical fuels with other methods of energy storage. For example, lithium ion batteries have energy densities on the order of 0.50 kJ/g. How does this compare with your fuels? What does it say about the relative advantage of fuels, especially in something like the transportation industry?

7) Very recently (Beller and co-workers *Nature* **2013**) there has been a report that methanol can be used as a medium for storing molecular hydrogen equivalents, which can be released via the following reaction known as "methanol reforming":



Suppose you have an equimolar mixture of methanol and water with density 0.885 g/mL. What is the molar volume of H2 in this mixture (in L solution/mol H2)? How does this compare with gaseous H2 at STP? Why might this be a desirable way to "store" hydrogen? Are there any disadvantages related to this method? How does this method compare with the direct use of methanol as a fuel?

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| --- | --- | --- | --- | --- |
| **Fuel** | **Energy Density (kJ/mol)** | **Energy Density (kJ/g)** | **Energy Density (MJ/L)** | **mmol CO2 per kJ heat produced** |
| Hydrogen (H2 (*g*)) |  |  |  |  |
| Coal (C (*s*)) |  |  |  |  |
| Natural Gas (methane, CH4 (*g*)) |  |  |  |  |
| Methanol (CH4O (*l*)) |  |  |  |  |
| Formaldehyde (CH2O, (*s*)) |  |  |  |  |
| Formic acid (CH2O2 (*l*)) |  |  |  |  |
| Propane gas (C3H8 (*g*)) |  |  |  |  |
| Liquid propane (C3H8 (*l*)) |  |  |  |  |
| Octane (C8H18 (*l*)) |  |  |  |  |