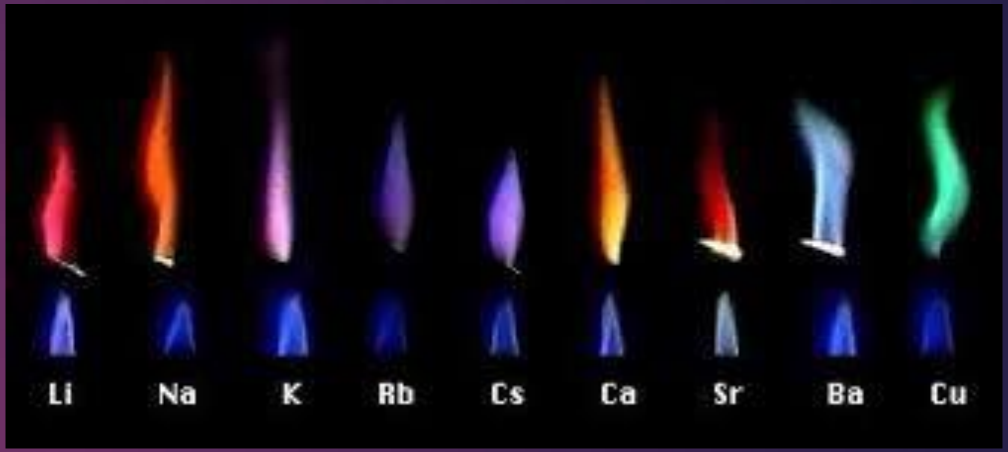
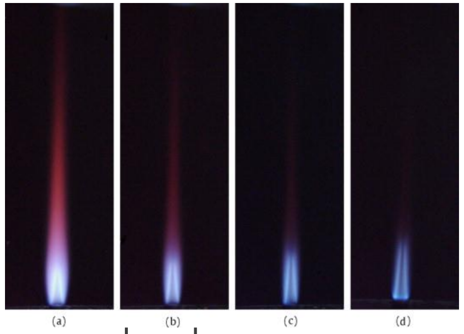


Combustion

THE SCIENCE OF FIRE AND RELATED PHENOMENA

The chemistry of combustion

- Result of a highly exothermic oxidation/reduction (redox) reaction.
  - Exothermic – heat is released with respect to the reaction, feels hot
  - Oxidation – Loss of electrons
  - Reduction – Gain of electrons
- Requires fuel and (usually) oxygen
- The simplest combustion reaction: $2H_2(g) + O_2 \rightarrow 2H_2O$
  - Oxygen acts the oxidizer by convention
  - Releases 242 kJ/mol of heat, as water is more stable than the reactants



The Steps of Combustion

- We will use wood as an example
- 1. Heating – The fuel needs to be heated so compounds inside can decompose and eventually reach activation energy
- 2. Pyrolysis – The breakdown and release of various compounds inside the fuel, depending on temperature
  - Below 100C – Free water starts to be released, and temperature sensitive compounds start to break down.
  - At or above 100C – Bound water starts to be released, this is the reason wood is hard to ignite. Temperature of the wood will remain at this point until all water is driven off, due to thermodynamics (heat of vaporization)

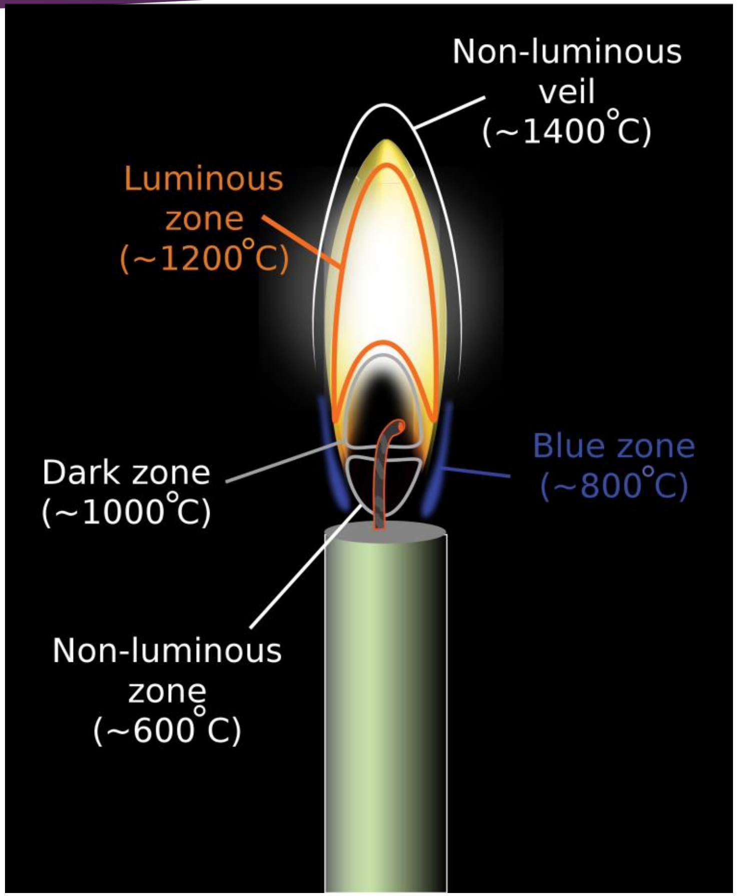
The Steps of Combustion (cont.)

- 2. Pyrolysis (cont.)
  - 100C – 500C – Other organic compounds start to decompose, creating smoke. Depending on the temperature, these may start a visible flame. It is possible to completely pyrolyze a fuel without igniting it (like coal for coke, or a pizza).
- 3. Combustion - Once a flame starts, this is the point where combustion takes over. The reaction is self sustaining, as additional fuel is undergoing pyrolysis.
- Completion – Any incombustible residue is manifested as ash

Fun fact: the composition of wood ash mostly consists of calcium compounds, either calcium carbonate or calcium oxide. The literature varies on this.

Types of Flame (for our purposes)

- Blue – Indicates complete combustion due to sufficient oxygen. Illumination caused by chemiluminescence, the emission of light from the reaction itself.
- Yellow – Incomplete combustion. Light comes from radiative emission by soot and complex free radicals like methlylidine (CH) and diatomic carbon.
- For both instances, the illumination is technically a plasma.
- A simple flame, as from a candle, is very complex and outside the scope of this presentation. There are hundreds of intermediary reactions.



Types of Combustion

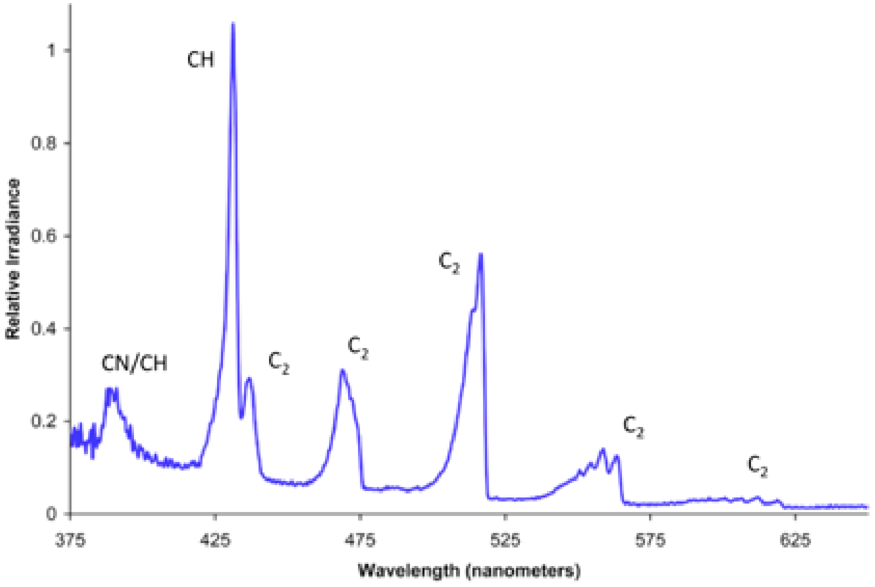
- Diffusion flame – The most common for everyday use. Fuel and oxidizer are separated before use. Ex. wood is separate from oxygen before burning
- Deflagration – subsonic combustion of a premixed fuel. Ex. gunpowder, smokeless powder.
- Detonation – supersonic combustion of a premixed fuel. Ex. C4 high explosive

Temperatures of Flame (Ideal)

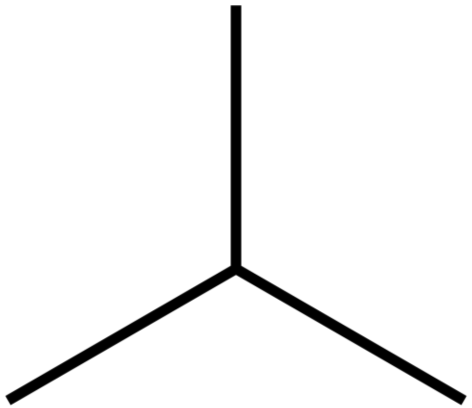
Fuel	Temperature (F)
Butane	3578
Charcoal	1382-2192
Propane blowtorch	2192-3092
Dicyanoacetylene	9010
MAPP gas	3668
Oxyacetylene	5972
Kerosene	1814
Gasoline	1878
Wood	1881
Coal	3590

Butane (C_4H_{10})

- 2 isomers, pictured right
- Discovered along with propane in 1912 by Dr. Walter Snelling
- Uses (other than burning) include:
  - Fragrance extraction
  - Synthetic rubber
  - Isobutane used to increase octane number in gasoline

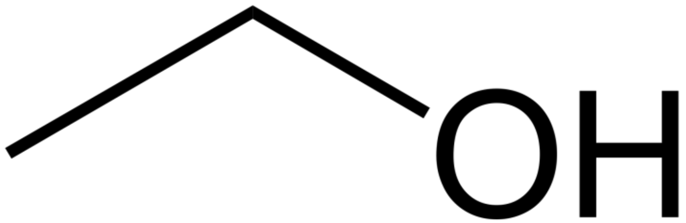


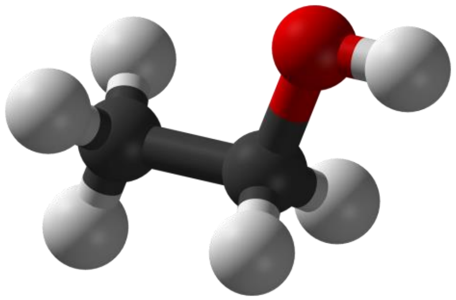
This is a spectral graph of a blue butane flame.



Ethanol (C_2H_5OH)

- Molecule looks like doggie
- Addition of hydroxyl group (OH) classifies it as an alcohol
- Lots of uses:
  - Solvent, disinfectant, industrial feedstock
  - Drinking
    - The antidote for methanol poisoning is ethanol





Coal (complicated)

- Classified as a sedimentary rock (like sandstone)
- Formed by decayed plant matter being compressed under high heat and pressure over millions of years
- Coal liquefaction
  - Used extensively by Germany during WW2 to produce gasoline via the Bergius process (hydrogenation, adding hydrogen)
  - Germany did not have any natural sources of crude

$$nC + (n+1)H_2 \longrightarrow C_nH_{2n+2}$$

Any Questions?