Chapter 5

Systems Thinking

Recap: what do we know? (expanded

- Atoms interact electrostatically – in a range from LDF to bonding (of all kinds)
- When atoms interact, the system becomes more stable (and loses energy to surroundings)
- All interactions require energy to overcome
- The way atoms interact depend on the arrangement of electrons (valence electrons)
- When atoms form new compounds the properties are emergent (not the sum of the atoms)
- Properties of materials depend upon the types of bonds and spatial arrangement of atoms
- Temperature of phase changes allows us to make

What is temperature?

- Measure of "hotness"
- Tells you which direction thermal energy will move (hot to cold – **why**?)
- Units Celsius °C, Kelvin K, (Fahrenheit °F)
- 0 °C = 273.15 K
- 0 K = absolute zero (lowest possible temp)
- A change of 1 °C = 1 K

Temperature and thermal energy?

- Thermal energy depends on how much material you have
  - (eg 1 drop of boiling water vs. a bucket of boiling water)
  - They have different thermal energies
- Temperature only depends on the average KE – so 1 drop or a bucket of boiling water still have the same T – but different amounts of thermal energy

Temp and Kinetic energy

- T is **directly** related to **average** kinetic energy ($1/2mv^2$)
- Can an individual molecule have a temperature?
- Do all the molecules move at the same speed at a given temperature? Why not?

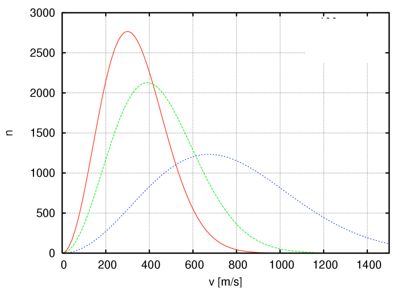
Populations vs individuals

- At the molecular scale we usually consider populations (ie a lot of particles)
- Populations of molecules can have a temperature where average KE = 3/2 kT (where k is a constant)
- ONE molecule can have a KE – but NOT a temperature
  - Temperature is a bulk property

Questions

- What happens to the average KE (or velocity) as the temperature increases?
- What happens to the average KE (or velocity) if we compare gases of different molar masses? (does a heavier gas move faster or slower?)
- When molecules collide why don't they stick together?
- The average speed of H_2 molecules is 2000m/s at 273K – why don't we smell things immediately?

Maxwell-Boltzmann distribution for a



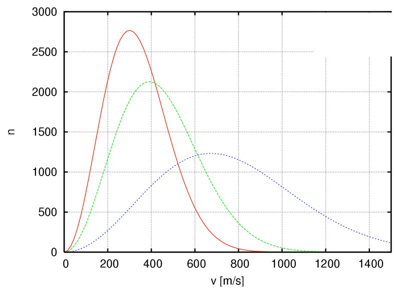
Which is at the highest T?

A. Red
B. Green
C. Blue

What about for different gases at the same T?

At a given temperature the average KE

Maxwell-Boltzmann distribution for different gases at the same temperature (Ne, Ar, Kr)



Which Kr?

A. Red
B. Green
C. Blue

Boltzmann

- KE = $1/2mv^2 = 3/2kT$
- k = Boltzmann's constant
- http://people.chem.byu.edu/rbshirts/research/boltzmann_3d
- (for a monatomic gas)

Values of *k*[1]	Units
$1.380\,6504(24) \times 10^{-23}$	$J\,K^{-1}$
$8.617\,343(15) \times 10^{-5}$	$eV\,K^{-1}$
$1.380\,6504(24) \times 10^{-16}$	$erg\,K^{-1}$
For details, see Value in different units below.	

Energy of motion

KE – normally associated with **movement** (translation)

But there are other forms of movement eg vibration and rotation that are important for more complex materials

Energy of Motion

Phase	Translation	Rotation	Vibration
Gas	Free	Free	Free
Liquid	Restricted	Less free than gas	Free
Solid	Absent	Very limited	Free

Heat and Thermal Energy

- Thermal energy – energy associated with motion of particles (Joules)
- Heat – strictly the transfer of thermal energy from one place to another (eg by collisions of molecules) –
  - Can tell which way it is transferred by the temperature (hot --> cold)

Specific heat/heat capacity

- How much energy it takes to change the temperature of a substance.
- Specific heat – energy required to raise 1 g by 1 °C (or 1 K)
- Molar heat capacity – energy required to raise 1 mol by 1 °C (or 1 K)

Name	Formula	Molar mass (g/mol)	Molar heat capacity (J/ mol	Specific heat (J/g °C)
water	H_2O	18	75.4	4.18
methanol	CH_3OH	32	81	2.53
ethanol	CH_3CH_2OH	48	112	2.44
propanol	$CH_3CH_2CH_2OH$	60	144	2.39

If you add the same amount of thermal energy to each of these, which one would increase in temperature most?

Propanol

What do you notice about the specific heat values shown?

So why is water so much higher?