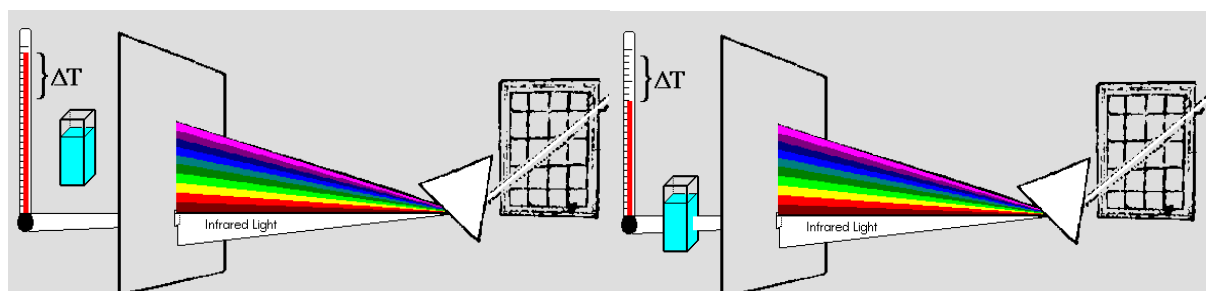
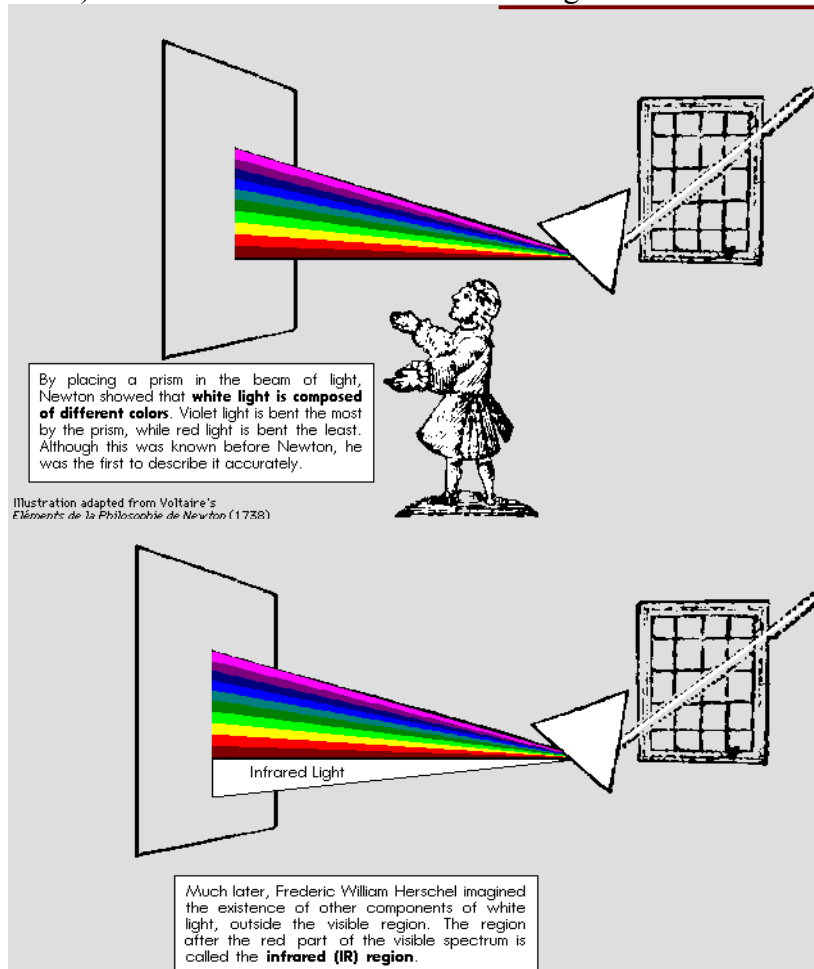


## Fragen zum IR-Programm

### Bereich : Introduction of spectroscopy

- 1.) F.W. Herschel entdeckte als erster die Bedeutung der IR – Strahlung für die Spektroskopie. Welche Experimente führte er durch?
- 2.) Wie verändert sich die Wellenlänge vom nahen zum fernen IR? Experimentieren Sie ein bisschen mit dem Programm und beobachten Sie die Veränderungen der Frequenz und Energie.
- 3.) Wie beeinflusst die IR-Strahlung die Moleküle?
- 4.) Wie ist ein einfaches IR – Gerät aufgebaut?



### Introduction to Spectroscopy

Wavelength

$$\lambda = 500.0 \mu\text{m}$$

Wavenumber

$$\bar{\nu} = 20 \text{ cm}^{-1}$$

Energy

$$E = 0.04 \times 10^{-20} \text{ J}$$

The **wavelength** of a beam of light defines its position in the electromagnetic spectrum. It is often more convenient to use the **wavenumber**  $\bar{\nu}$ , defined as the inverse of the wavelength. The **energy** of the light is related to its wavelength by the formula  $E = hc/\lambda = hc\bar{\nu}$ , where  $h$  is Planck's constant ( $6.62 \times 10^{-34} \text{ J}\cdot\text{s}$ ).

**Drag the indicator bar (far left) up and down.**

### Introduction to Spectroscopy

Wavelength

$$\lambda = 1.1 \mu\text{m}$$

Wavenumber

$$\bar{\nu} = 9000 \text{ cm}^{-1}$$

Energy

$$E = 17.9 \times 10^{-20} \text{ J}$$

The **wavelength** of a beam of light defines its position in the electromagnetic spectrum. It is often more convenient to use the **wavenumber**  $\bar{\nu}$ , defined as the inverse of the wavelength. The **energy** of the light is related to its wavelength by the formula  $E = hc/\lambda = hc\bar{\nu}$ , where  $h$  is Planck's constant ( $6.62 \times 10^{-34} \text{ J}\cdot\text{s}$ ).

**Drag the indicator bar (far left) up and down.**

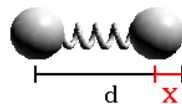
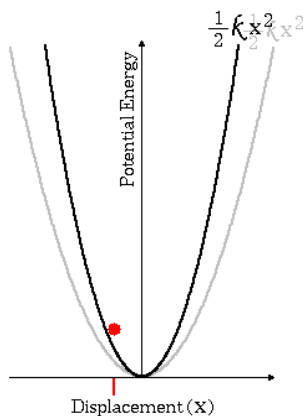
## Bereich: Theory of IR

- 1.) Um sich vorstellen zu können, wie sich Moleküle bei IR-Strahlung verhalten, gibt es verschiedene Modelle. Die Einfachste ist das Federmodell (spring =Feder). Versuchen Sie herauszufinden, wie sich die Frequenz ändert wenn es sich um:
  - große bzw. kleine Massen handelt
  - starke und schwache Bindungen.
  
- 2.) Das Modell der Feder trifft allerdings nicht ganz zu. Während man sich bei der Feder beliebige Energiemengen vorstellen kann, ist die Energieaufnahme bei Molekülen begrenzt.  
Warum kann die Energie nur portionsweise aufgenommen werden und warum gibt es ein Energielimit? (Hilfe : durch Ausprobieren des interaktiven Teils bekommen Sie Infos).
  
- 3.) Welche Bedingung muss ein Molekül mitbringen um IR-aktiv zu sein ?
  
- 4.) Was versteht man unter Fingerprintbereich?



### Model of a Simple Molecule

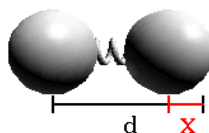
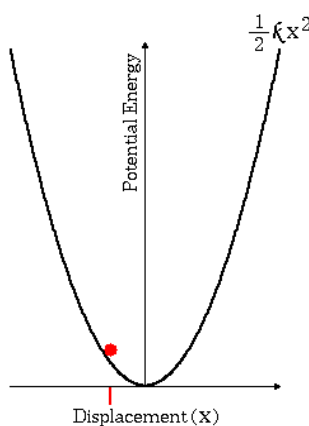
A diatomic molecule can be modelled by a spring with force constant  $k$  attached to two balls of mass  $m$ . This is called the **classical harmonic oscillator** model.



The **vibration frequency**  $\nu$  is related to the force constant  $k$  and mass  $m$  by the equation:

$$\nu = \frac{1}{2\pi} \sqrt{\frac{k}{m}}$$

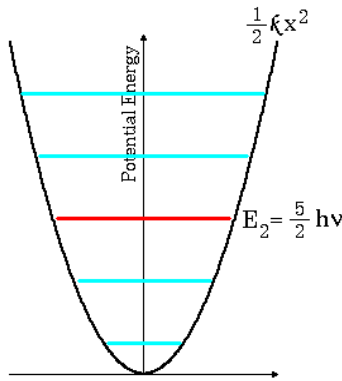
Therefore, a larger force constant (stronger spring) results in a higher frequency...



$$\nu = \frac{1}{2\pi} \sqrt{\frac{k}{m}}$$

A larger mass results in a lower frequency, but the potential energy curve does not change.

## Theory of Infrared Spectroscopy

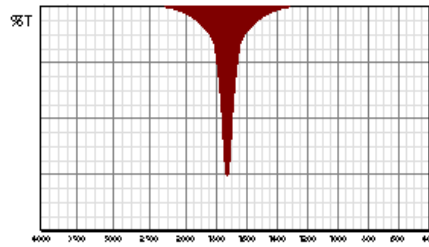
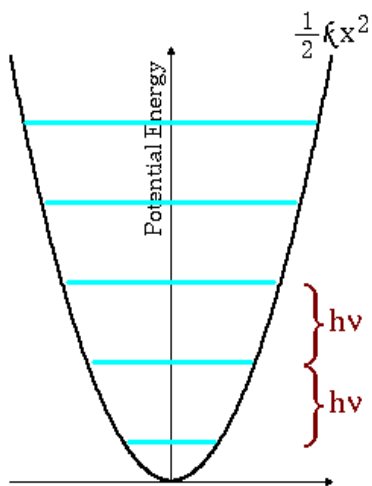


In the quantum mechanical model, a molecule may only absorb (or emit) light of an energy equal to the spacing between two levels. Furthermore, for a harmonic oscillator these transitions can only occur from one level to the next higher (or lower) level, i.e.  $\Delta n = \pm 1$ . This is called the **selection rule**. Press the buttons below to see absorption and emission:

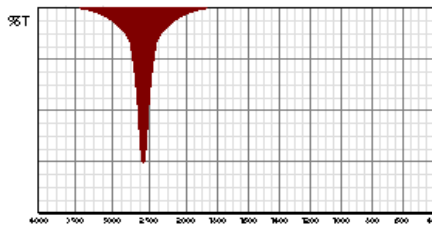
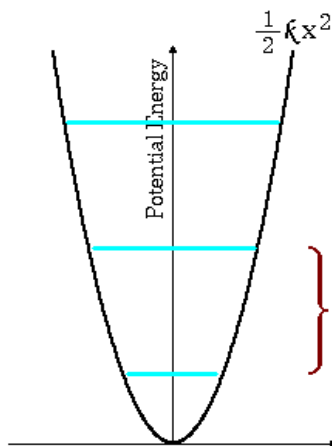
Absorb

Emit

(The molecule would break apart if it absorbed more energy)

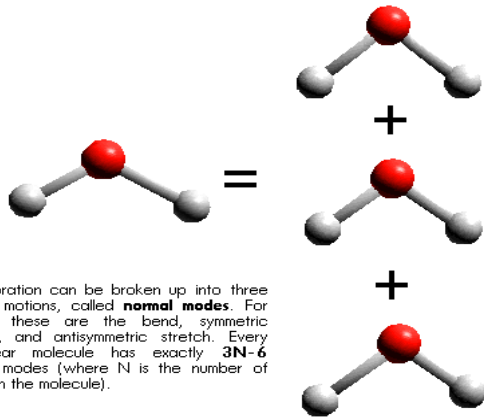


Because of the selection rule, a molecule can only absorb light with energy equal to  $hv$ . Therefore, the infrared spectrum of this molecule should have a single peak at the frequency corresponding to that energy.

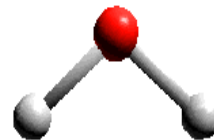
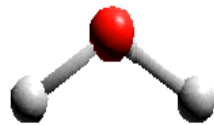
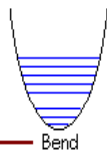
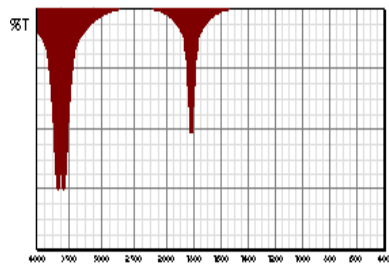


A higher frequency (due to a larger force constant or a smaller mass) results in a larger spacing between the levels ... and a lower frequency results in a smaller spacing between the levels.

(Click on the arrow above)



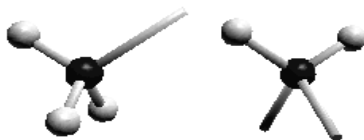
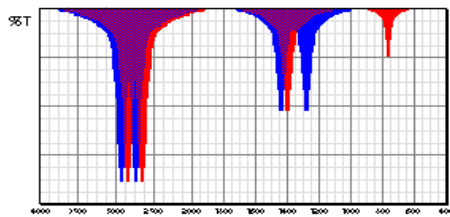
The vibration can be broken up into three simpler motions, called **normal modes**. For water, these are the bend, symmetric stretch, and antisymmetric stretch. Every non-linear molecule has exactly  $3N-6$  normal modes (where N is the number of atoms in the molecule).



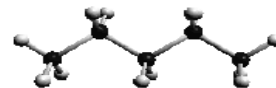
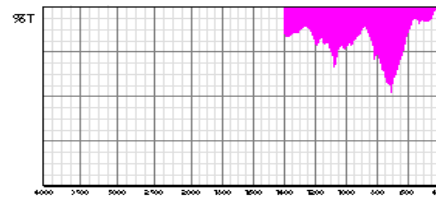
Symmetric Stretch

Antisymmetric Stretch

Since each normal mode has a change in dipole moment as it vibrates, each will absorb infrared light. Three peaks should appear in the infrared spectrum of water. Note that the two stretching vibrations overlap.



Each functional group therefore has a set of **group frequencies** which correspond to the normal modes for the group.



Peaks below 1400  $\text{cm}^{-1}$  are part of the so-called **fingerprint region**. Many of the bands observed in this region are dependent on the overall molecular structure rather than individual functional groups. The pattern in this region is therefore very specific for a molecule and comparison with a reference spectrum can positively identify a compound.

The remaining sections of the program are fully interpreted infrared spectra. Click on the double arrow to begin with Hexane

### **Bereich: Interpretation of spektra**

Dieser Bereich ist besonders wichtig weil Sie hier beobachten können, wie die einzelnen Gruppen schwingen.

- 1.) Vergleichen Sie Hexan mit Cyclohexan (mit Overlay). Welche Unterschiede stellen Sie fest ?
- 2.) Warum findet man bei hohen Wellenzahlen Valenzschwingungen (=hier stretching) und in niedrigen Bereichen Deformationsschwingungen (= hier bending) ?
- 3.) Vergleichen Sie Hexylamin mit Tributylamin. Welche Unterschiede stellen Sie fest ?
- 4.) Im Programm ist das Molekül Toluol enthalten. Interessant ist für uns der Grundkörper: das Benzol. Welche typischen Schwingungen findet man ?