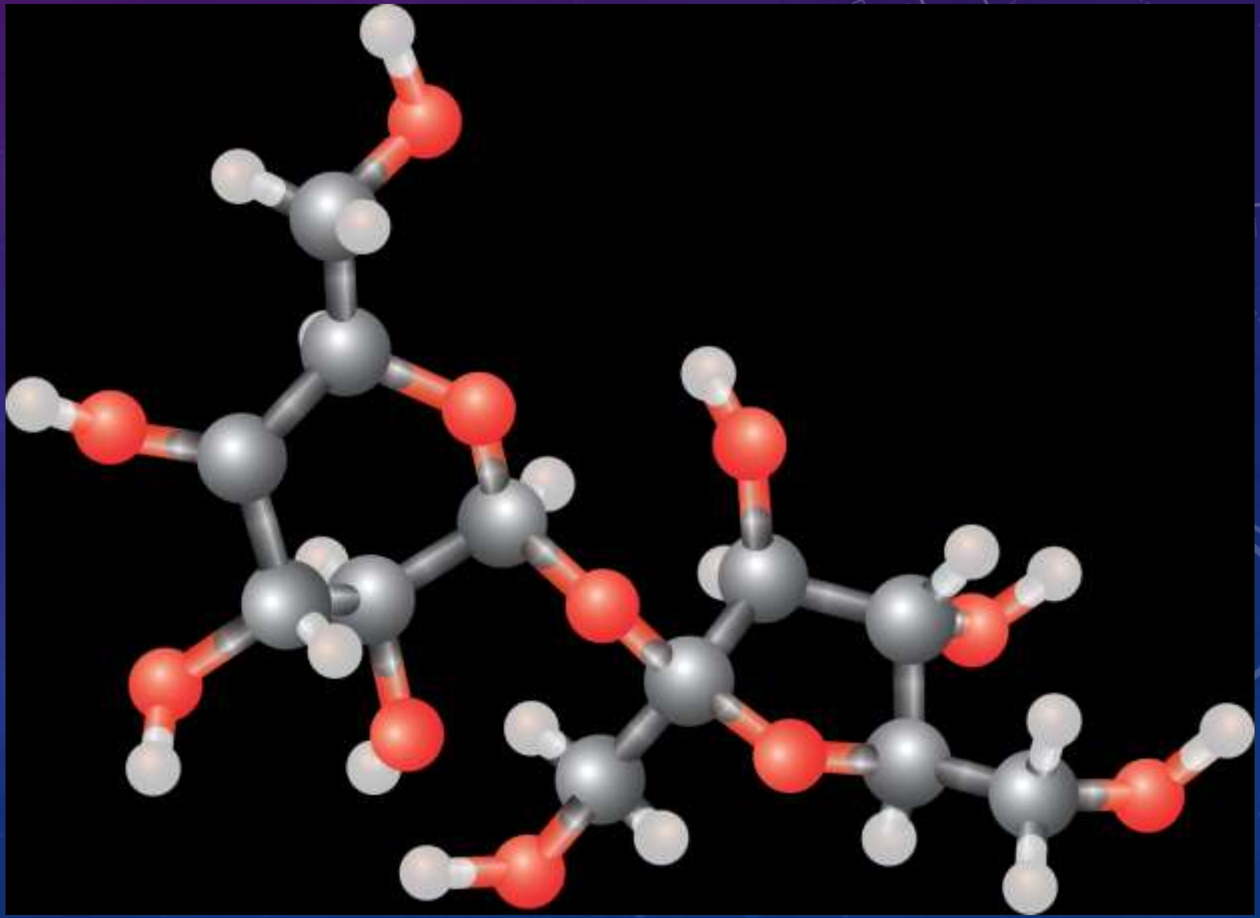
SPECTROSCOPY:
IR AND NMR

BECKY HAIGHT, MATH 198

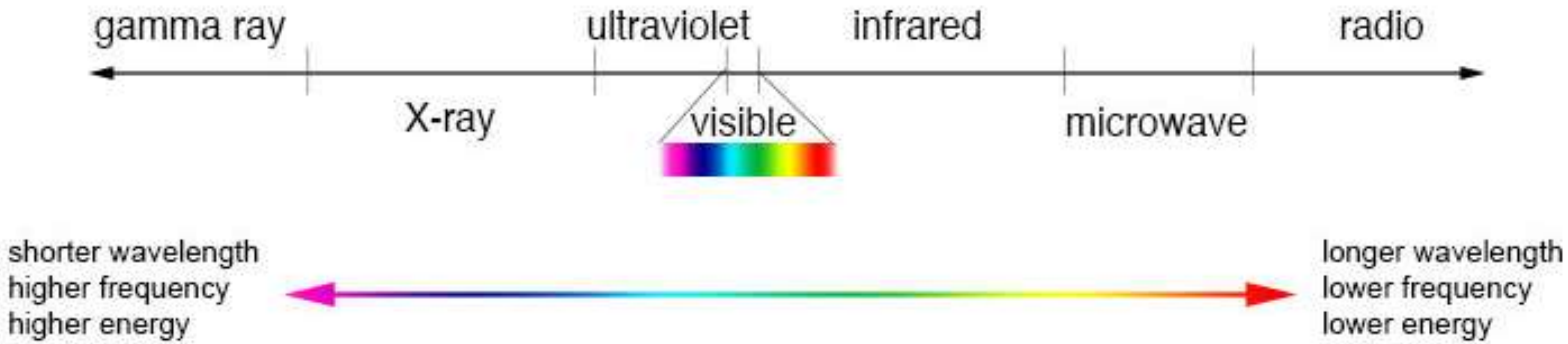
PROJECT OVERVIEW

- Learn some basic programming language
    - VPython
- Create a simple carbene (CH_2) model
- Demonstrate various vibrational modes of IR
- Understand difference between IR and NMR



SPECTROSCOPY: AN INTRODUCTION

- Spectroscopy in chemistry is the study of the interactions between molecules exposed to light
- $\Delta E = hf = \frac{hc}{\lambda}$
- $c = f\lambda$

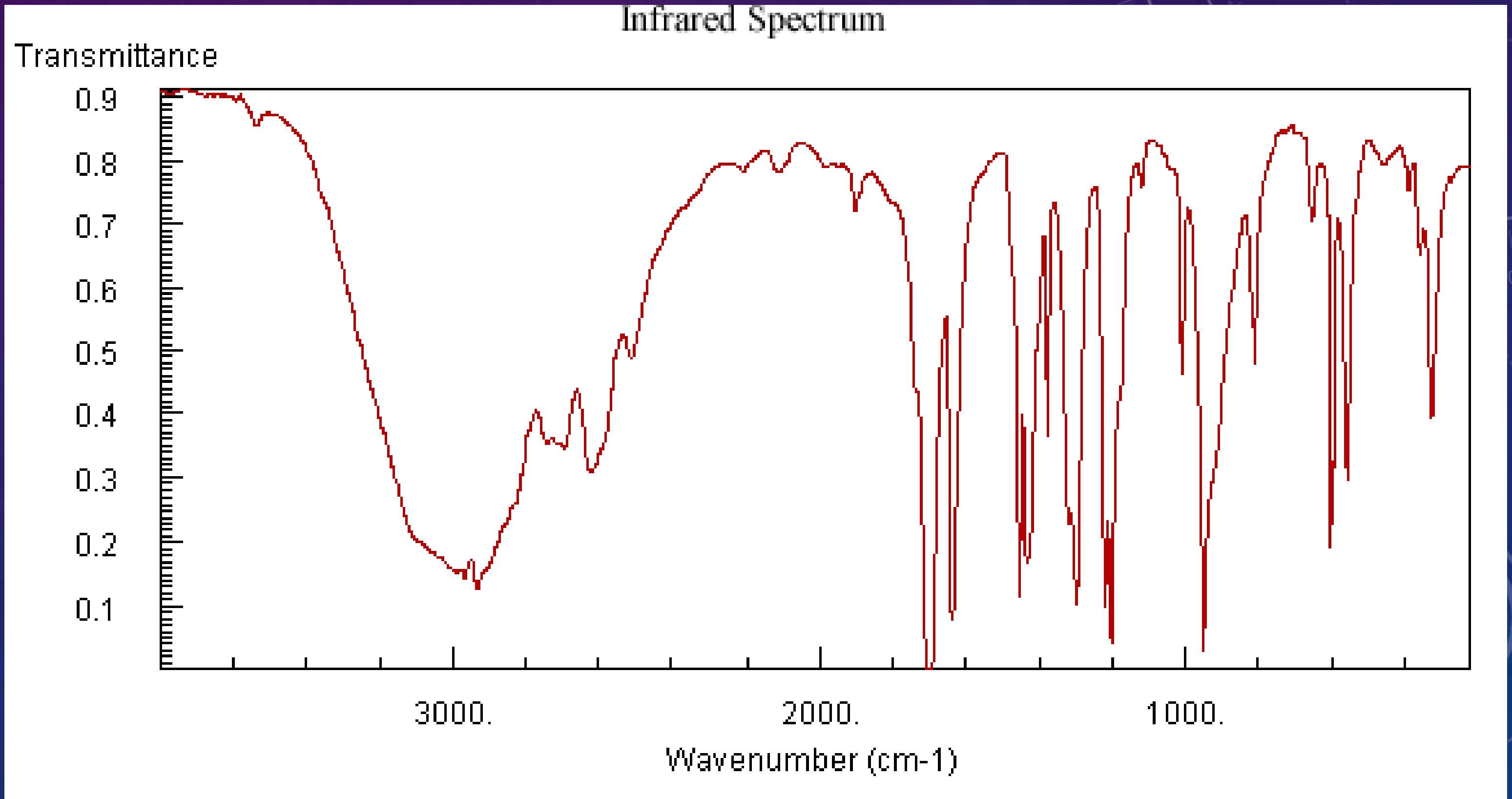


INFRARED SPECTROSCOPY

- Infrared radiation: long wavelength, low frequency
- Different ranges:
  - Near-IR
  - Mid-IR (most widely used region)
  - Far-IR
- Qualitative data: Functional groups

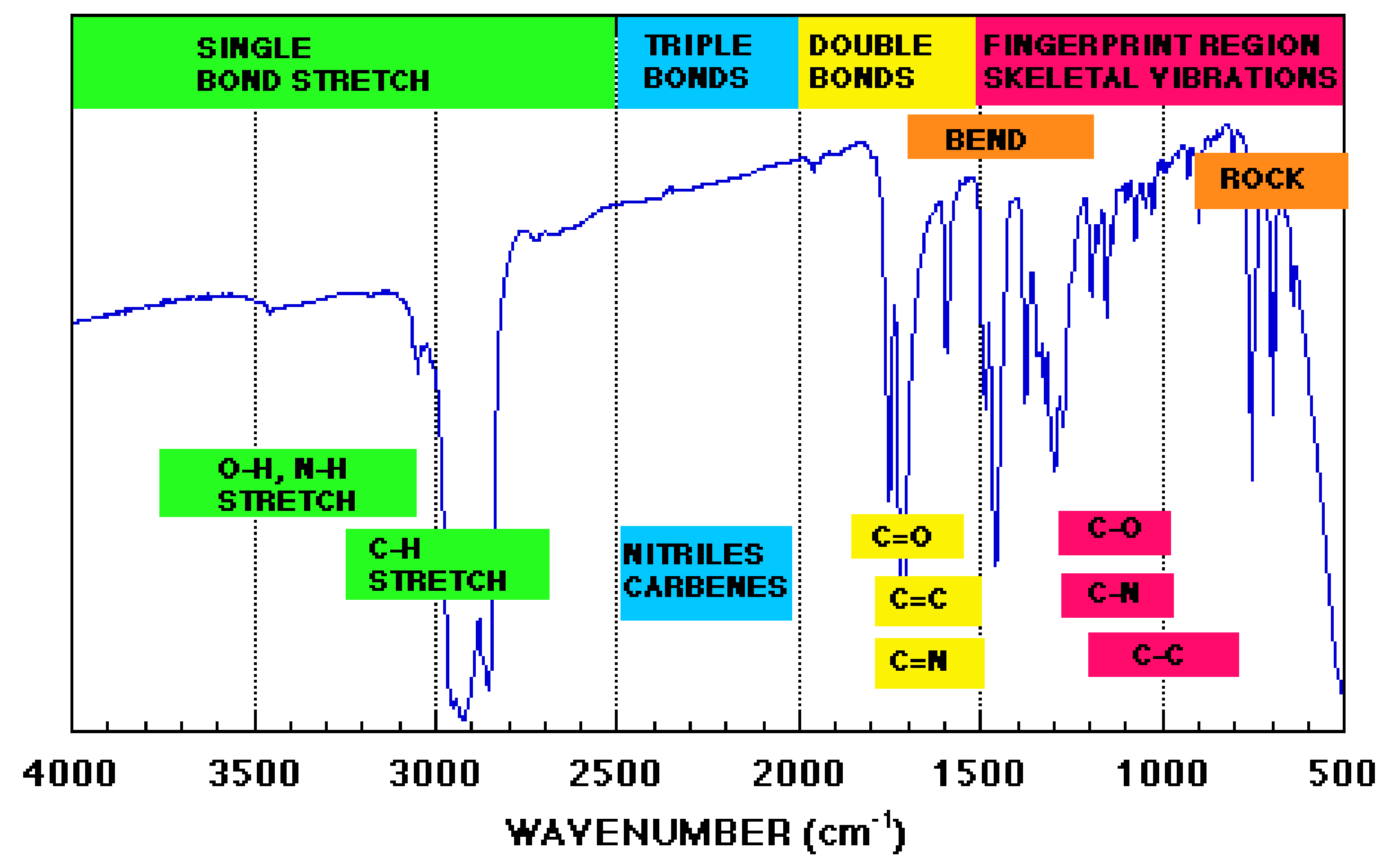
INFRARED SPECTROSCOPY: SPECTRUM AXIS

- X-Axis: Wavenumber (cm^{-1})
- Y-Axis: Percent transmittance
    - Dipole moment
    - Peak intensity



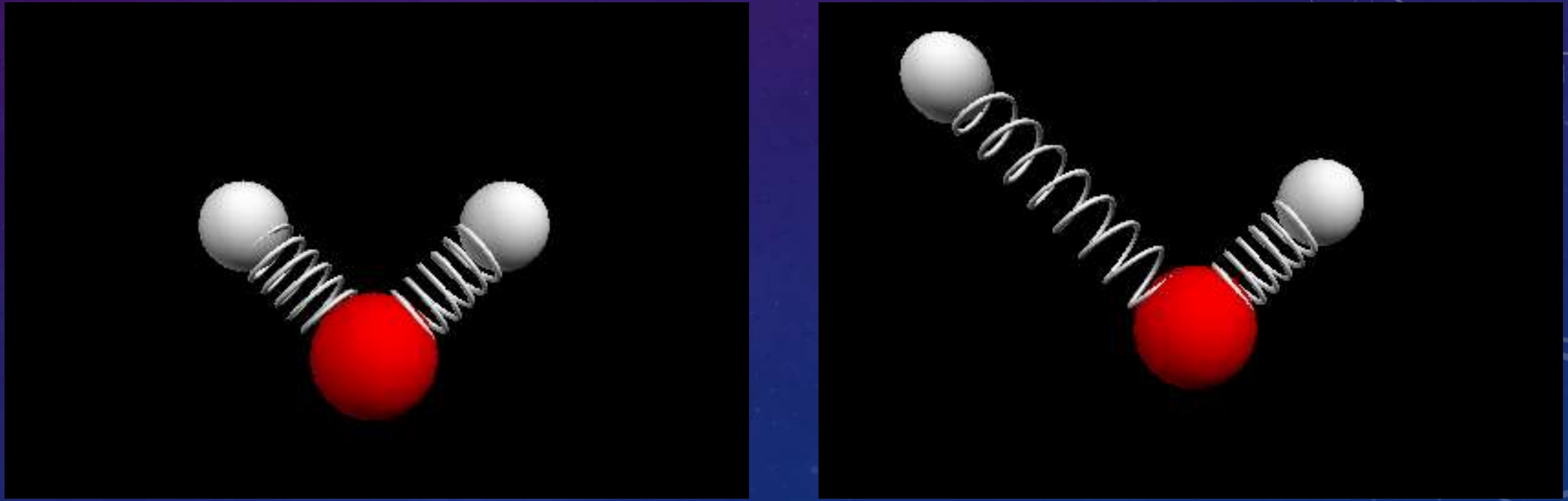
INFRARED SPECTROSCOPY: SPECTRUM

- Determining wavenumber
  - $\bar{\nu} = \frac{1}{\lambda}$
  - $\bar{\nu} = \frac{1}{2\pi c}\sqrt{\frac{k(m+M)}{mM}}$
- Highly sensitive
- Fingerprint region (<1500cm^{-1})



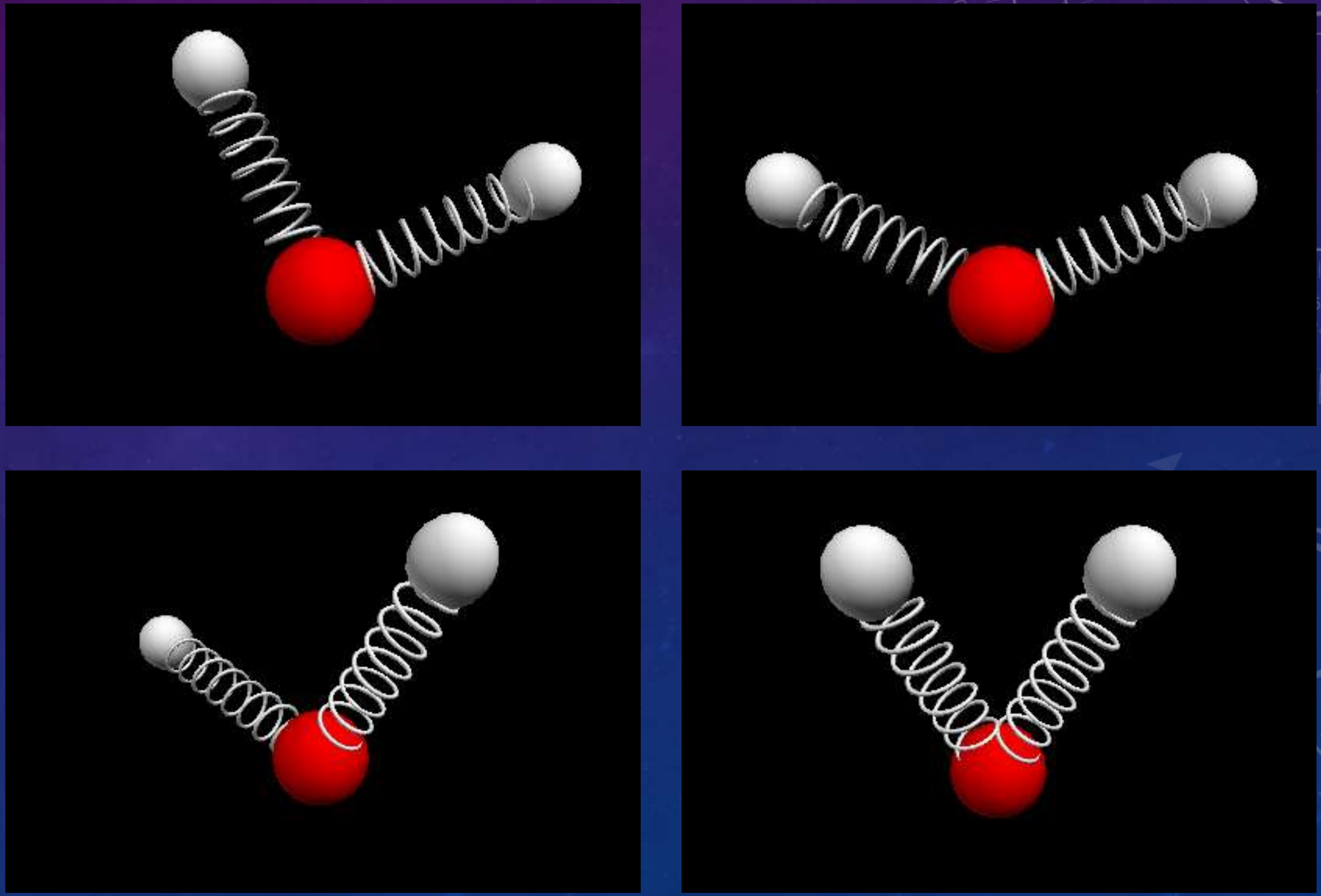
INFRARED SPECTROSCOPY: STRETCHES

- Occurs along line of bond
- Higher in energy
- Usually two peaks:
    - Symmetric
    - Asymmetric



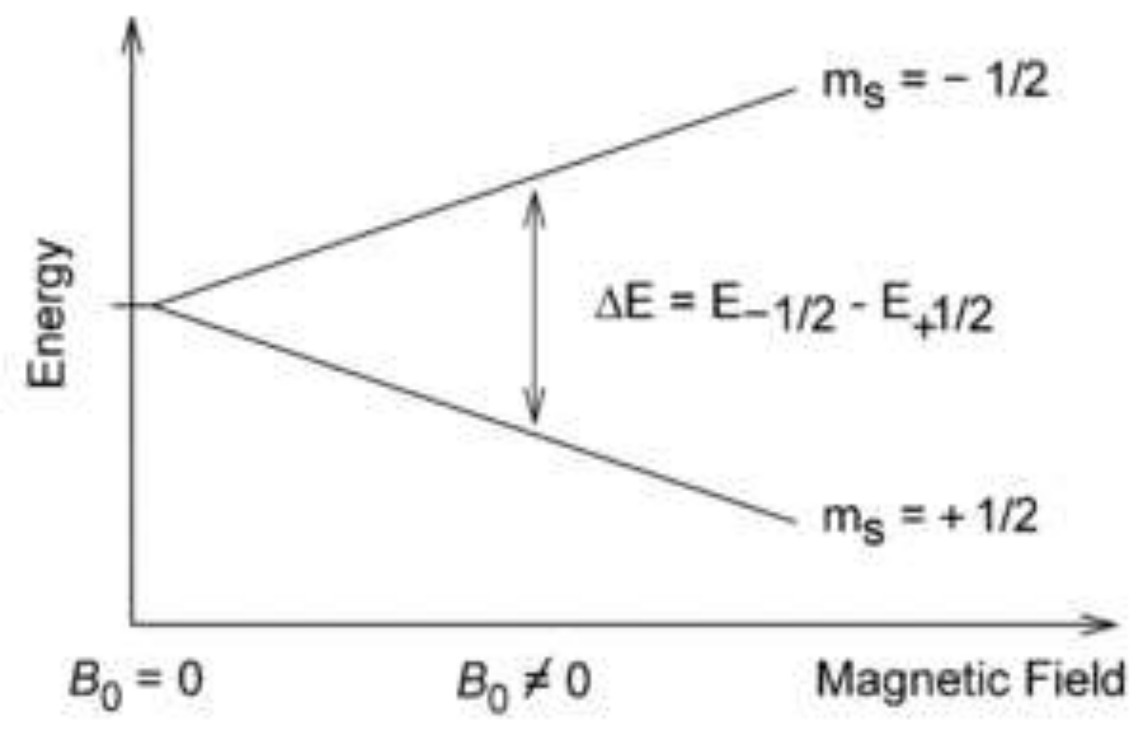
INFRARED SPECTROSCOPY: BENDS

- Any vibration not along line of bond
- Lower in energy
- Normal vibrational modes:
    - Rocking
    - Scissoring
    - Twisting
    - Wagging
- Many fall in fingerprint region



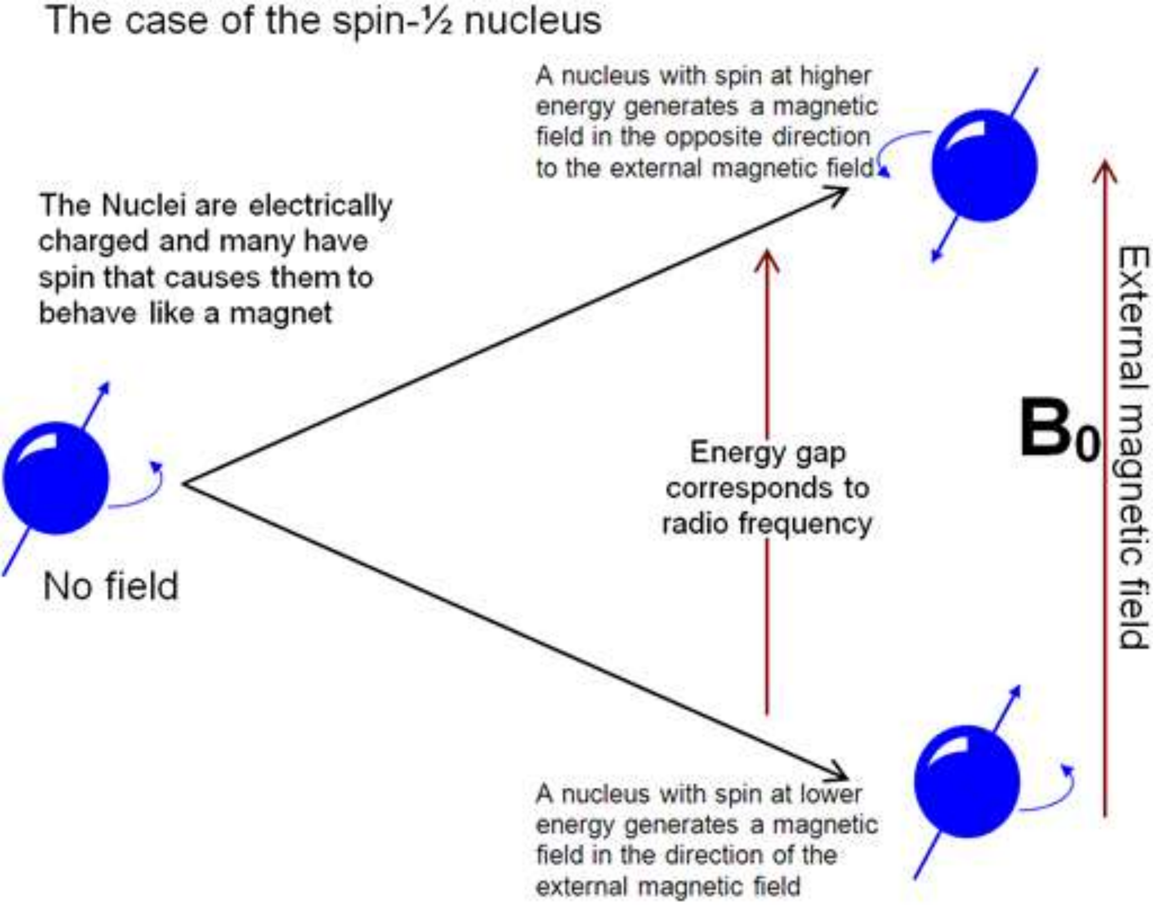
NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

- Radio waves: longer wavelength, higher frequency
- Magnetic field
- Nuclear spin
  - Any nucleus with an odd number of protons and electrons
  - Possible nuclei: ^{1}H, ^{13}C, ^{15}N, ^{19}F
- Qualitative and quantitative data: Molecular structure



NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

- Fundamental equation of NMR: $\Delta\epsilon_p = \frac{h\gamma_H}{2\pi}\boldsymbol{B_o}$
  - $\Delta\epsilon_p$: energy difference between spin states
  - γ_H: gyromagnetic ratio
  - $\boldsymbol{B_o}$: magnetic field magnitude at proton



The case of the spin-½ nucleus

A nucleus with spin at higher energy generates a magnetic field in the opposite direction to the external magnetic field

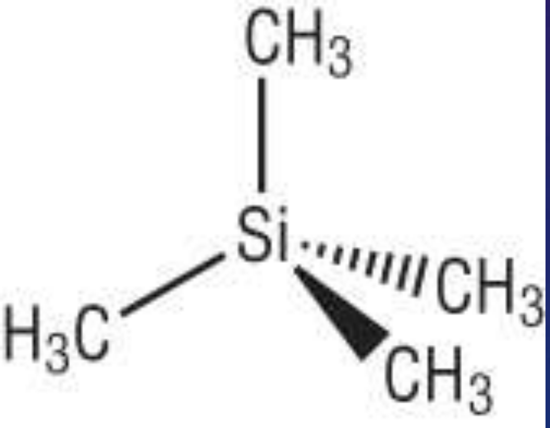
The Nuclei are electrically charged and many have spin that causes them to behave like a magnet

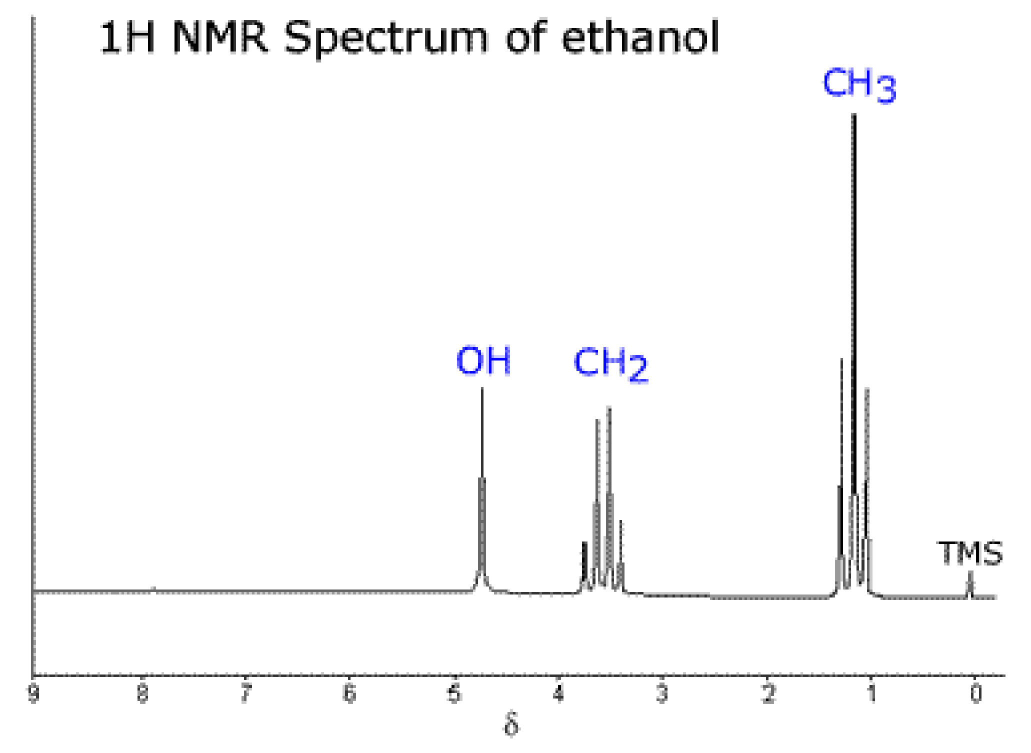
Energy gap corresponds to radio frequency

A nucleus with spin at lower energy generates a magnetic field in the direction of the external magnetic field

NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY: SPECTRUM

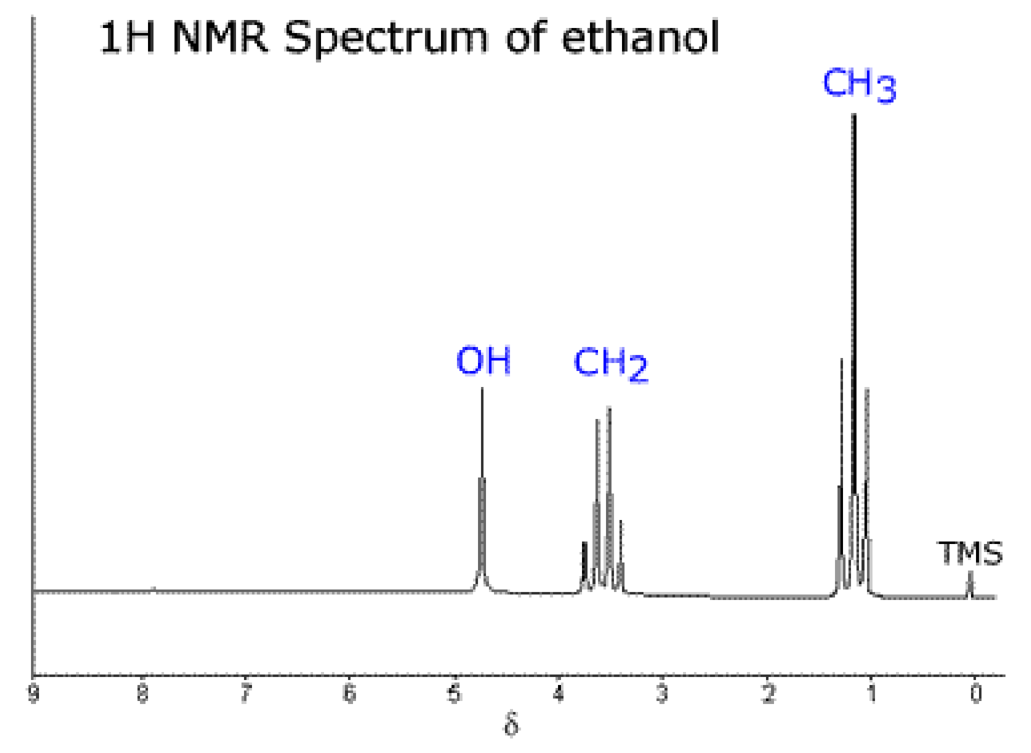
- X-Axis: Chemical shift (ppm)
- Tetramethylsilane (TMS)
- Solvent ($CDCl_3$)



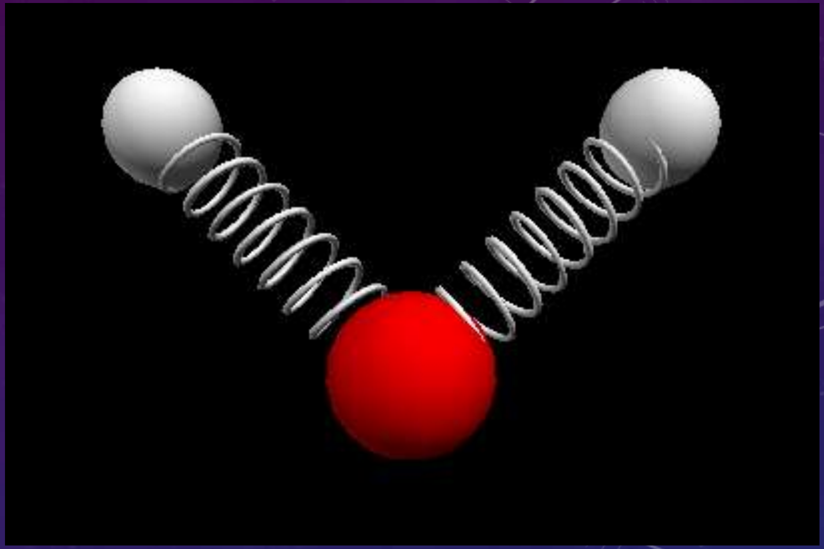


NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY: PROPERTIES

- Chemical shift (ppm): δ
  - Upfield vs downfield
  - Shielding vs deshielding
- Multiplicity
  - J-coupling (Hz)
  - Splitting is n+1
- Integration
  - Ratio



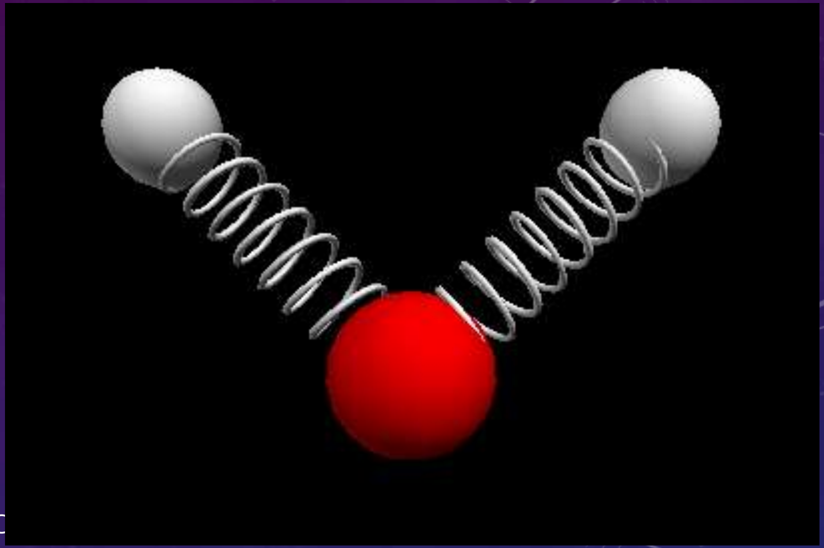
CODE: FRAMES



Set the frames of the hydrogens relative to that of carbon:

```
fcarbon = frame()
fhydrogen1 = frame(frame=fcarbon, pos=(3,3,0))
fhydrogen2 = frame(frame=fcarbon, pos=(-3,3,0))
```

CODE: OBJECTS



Used spheres to create the atoms:

```
carbon = sphere(frame=fcarbon, pos=(0,0,0), radius=1, c
```

```
hydrogen1 = sphere(frame=fhydrogen1, pos=(0,0,0), radius=0.7,
color=color.white)
```

```
hydrogen2 = sphere(frame=fhydrogen2, pos=(0,0,0), radius=0.7,
color=color.white)
```

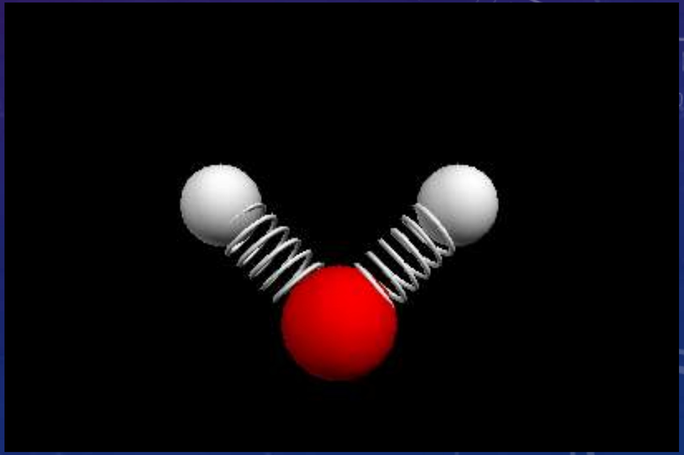
And helixes to create the bonds:

```
bond1 = helix(frame=fcarbon, pos=carbon.pos,
axis=(fhydrogen1.pos.x,fhydrogen1.pos.y,fhydrogen1.pos.z), coils=10,
thickness=0.1, radius=0.5)
```

```
bond2 = helix(frame=fcarbon, pos=carbon.pos,
axis=(fhydrogen2.pos.x,fhydrogen2.pos.y,fhydrogen2.pos.z), coils=10,
thickness=0.1, radius=0.5)
```

CODE: INFINITE LOOP

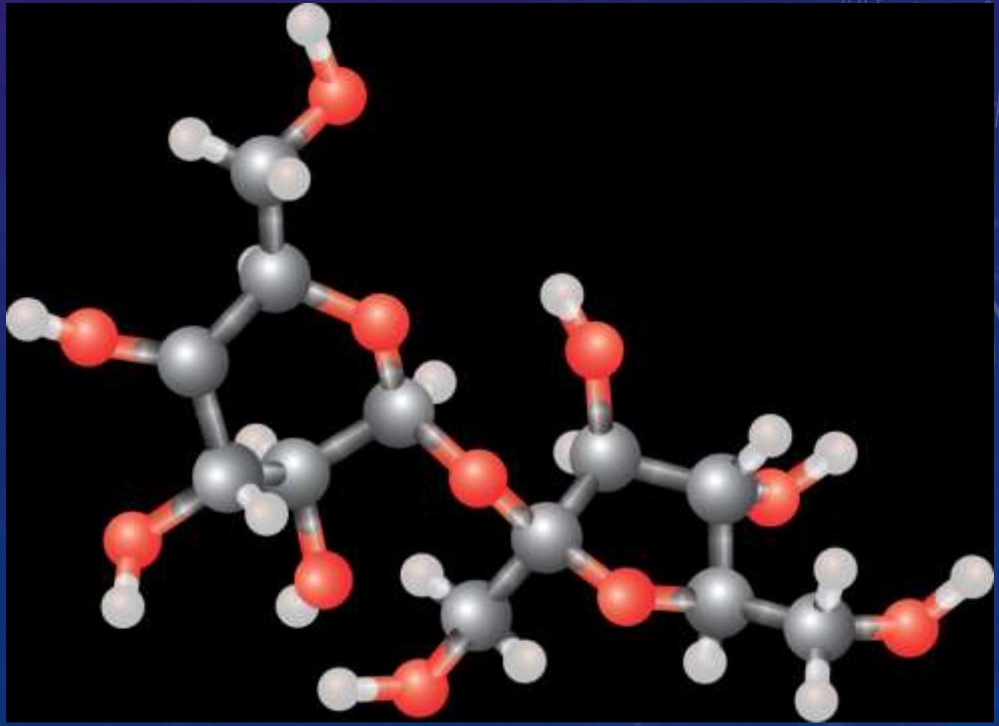
Each movement was different but set up similarly with an infinite while loop. Using a sine function to create the oscillating or rotating motion, it was simply a matter of moving the along the correct axis. The code for the symmetric stretch is given below:



```
t=0
br=1
while 1:
    rate(50)
    t=t+0.1
    fhydrogen1.pos=(3+br*sin(t),3+br*sin(t),0)
    bond1.axis=(fhydrogen1.pos.x,fhydrogen1.pos.y,fhydrogen1.pos.z)
    fhydrogen2.pos=(-3-br*sin(t),3+br*sin(t),0)
    bond2.axis=(fhydrogen2.pos.x,fhydrogen2.pos.y,fhydrogen2.pos.z)
```

FUTURE IMPROVEMENT AND EXPANSION

- Create more complex models
  - Carbon chains
  - Compare different types of bonds between different types of atoms
    - User interactive
- For the RTICA itself
  - Combine all the modes on one code



REFERENCES AND ACKNOWLEDGEMENTS

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