

## Electron in a Molecular Box

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### Practical:

Molecules with extensive pi bonding systems, like benzene, are often planar, or largely planar, and two types of bond contribute to their structure, sigma bonds and pi bonds. The sigma bonds are to be thought of as *localized* between atoms, whilst the pi bonds are to be thought of as being *delocalized* over large portions of the molecule. Much of the interesting chemistry of such compounds appears to relate to the so-called pi electrons, and we think about these pi electrons moving in a potential caused by the nuclear framework and the sigma electrons.

From the early days of quantum chemistry, people have striven to give simple models of such compounds in an effort to

- explain the special structure, stability and properties of these molecules, and
- to predict new properties of new molecules.

In this experiment, you use a spectrophotometer to measure the absorption spectrum of a conjugated molecule. You then predict the absorption spectra of two related molecules and compare your predictions with experiment.

### Intended academic level

Level 1

### Duration

6 hours (including write up)

### Outcomes

To illustrate the operation of a simple spectrophotometer by measuring the visible absorption of a conjugated molecule

To use the 'electron in a box' model in order to correlate the electronic spectra of three related conjugated molecules.

### Materials

White coat, safety goggles. Simple spectrophotometer. Dyestuff or something similar, part of a conjugated series. Ask the synthetic chemists for help or buy cyanine dyes from Kodak

### Costs

Next to nothing, assuming availability of spectrophotometer

### **Further comments**

Used successfully at UMIST for many years

### **Reading**

Chemical principles, the quest for insight. Peter Atkins, Loretta Jones (1999), New York: W.H. Freeman (section 1.5)

### **Contact details**

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