Aldehyde Monolayers by Chris Halcrow with support from Dr Stuart Clarke

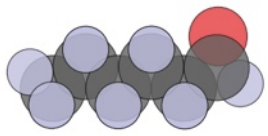
Experimental evidence has shown that when aldehydes are absorbed onto graphite a solid monolayer is formed. The structure of these monolayers can be examined by comparing scattering data with theoretical models. The project requires many aspects of mathematics, including statistics, optimisation, arithmetic trickery, computational work and density functional theory.

Some aspects of the project are discussed below

The Structure

Since a monolayer is formed, we are dealing with a two dimensional problem.

The basic building block is similar for any aldehyde.

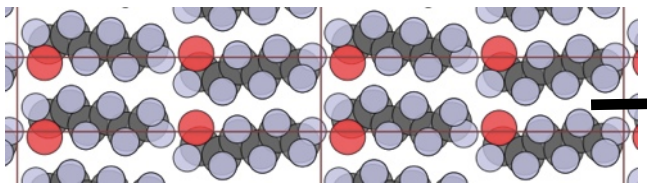


Hexanal (C6) - a building block

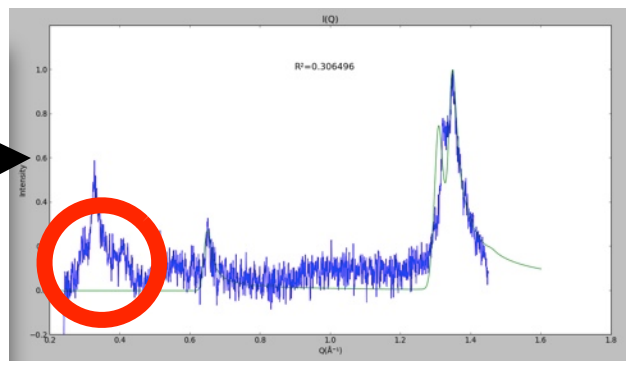
There are 17 symmetry groups, giving rise to many different scattering patterns.

Some examples:

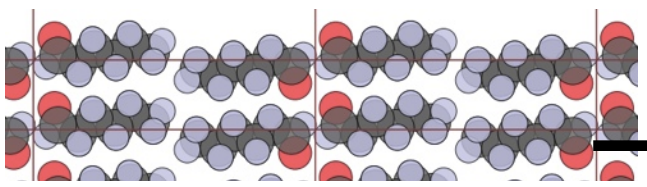
pga symmetry



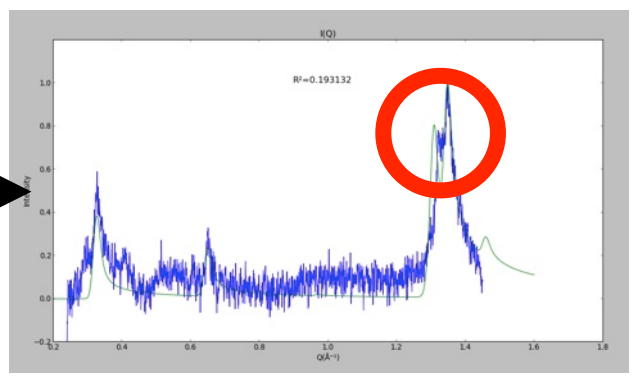
Can be ruled out due to lack of the first peak



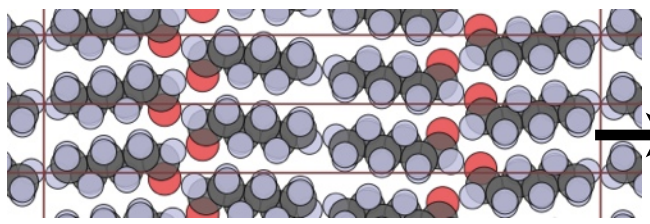
p2 symmetry



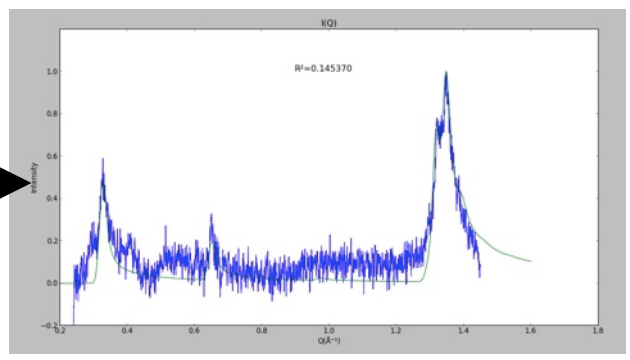
Double peak does not match using this symmetry group



pgg symmetry

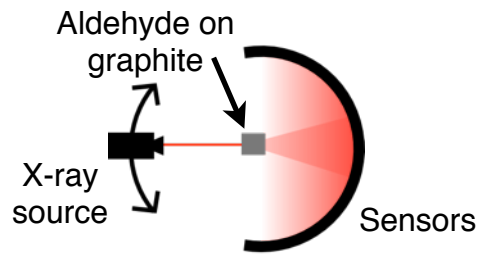


Fits all peaks - the only matching symmetry group for hexanal



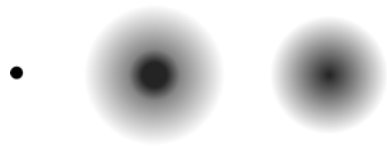
Experimental Aspect

All data (blue in graphs below) is from the Diamond Light Source or the Paul Sherrer Institute, using roughly the set up below.

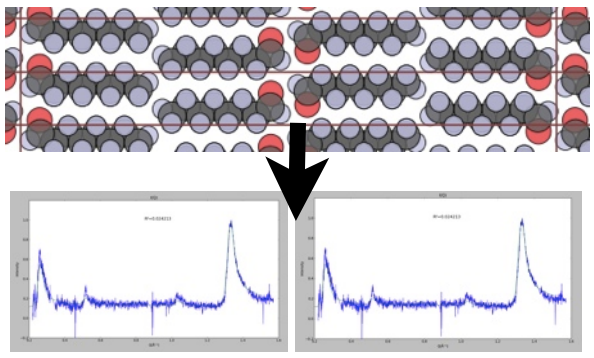


The Line shape

In a 2D model, reciprocal space is littered with Bragg peaks. In an ideal world, these are modeled as Dirac delta functions. In real life, should we model these as gaussian or lorentzian peaks?



Both can provide excellent fits, without any changes in the structure of the aldehyde

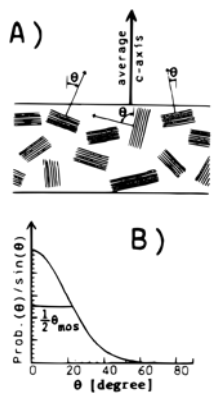


But can we statistically distinguish between these? Difficulties include:

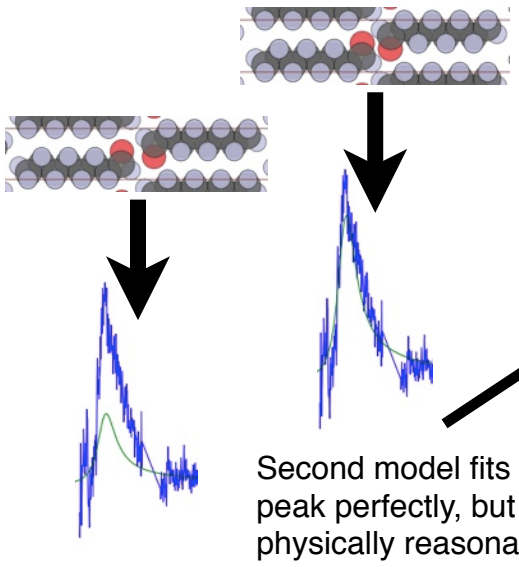
- Error *not* normally distributed
- Many outliers
- Possible inaccuracies of initial peak and final tail measurements

Non isotropic powder

The aldehyde powder is not isotropic, the orientation distribution (left) adds another complication to the theoretical model.



Realistic Models and Further Work

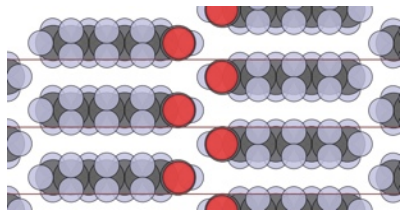


Second model fits this peak perfectly, but is it physically reasonable?

D F T

Density Functional Theory can tell us which models are energetically favored and which are physically impossible.

Calculations require much technical know how and a supercomputer



There is little difference between the output of the chains when they are flat in the plane (below), or perpendicular (above). How do we know which is the correct answer?