# Key Stage 3 – Crystal Modelling

## Pupil worksheet

### X-ray crystallography

What is inside a crystal of salt? How are atoms arranged to make the protein molecules of your heart? What is Mars made of?

How do scientists answer these questions? They use X-ray crystallography. Just as doctors use X-rays to see bones in your body, scientists use X-rays to look into crystals. If an X-ray crystallographer can obtain crystals of a substance, she or he can find out how its atoms are arranged.

### Your task

X-ray crystallography is a vital technique. Can you explain it to someone else?

**Preparation**

- Read the section *How X-ray crystallography works*.
- Look at models A to J. Some are pictures or ideas. Others are things you can hold or try out.
- Work out which stage of X-ray crystallography each model helps to explain. Some stages have more than one model. Some models help explain more than one stage.
- Choose five or fewer models. Plan how to use the models to explain what X-ray crystallography is, how it works, and why it is important.

**Explanation**

- Present your explanation to students from another class.
- Be prepared! The students will use the peer evaluation sheet to assess you.



### How X-ray crystallography works

Scientists use X-ray crystallography to work out the arrangement of atoms in a substance.

**Stage 1**

Make a crystal of the substance. The crystal must be very pure and perfect.

**Stage 2**

Fire X-rays at the crystal. The X-rays change direction as they go through the crystal. This is diffraction. Diffraction produces a pattern of spots. Some spots are more intense (darker) than others. Every type of crystal makes its own pattern of spots.

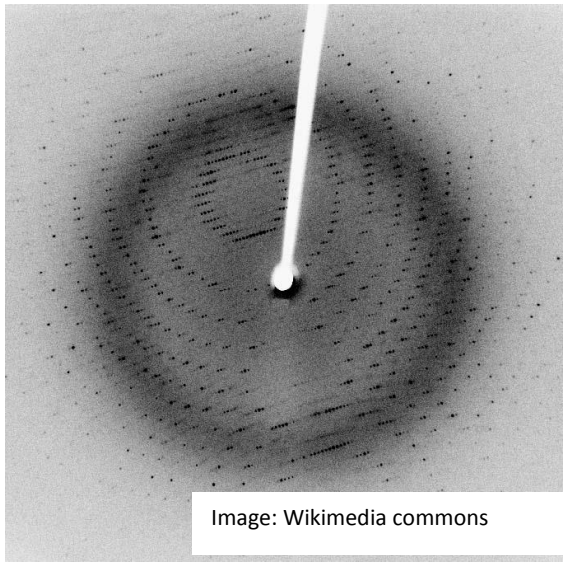


Image: Wikimedia commons

**Stage 3**

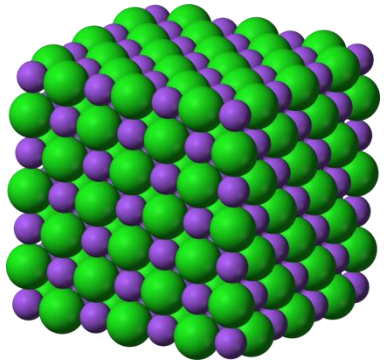
Continue to fire X-rays at the crystal whilst rotating the crystal a small amount, say 1°. Repeat until the crystal has turned through at least 180°. This results in up to 180 diffraction pattern images of the crystal.

**Stage 4**

Use a computer program (and lots of skill) to produce a 3D picture of the crystal structure from the many 2D diffraction pattern images.

# Key Stage 3 – Crystal Modelling

## Model A - spheres



You can use spheres to represent atoms in a crystal. This is a model of sodium chloride (salt.)

Key:
purple = sodium
green = chloride

Can you make a model crystal?

## Model B - soldiers

Each line of soldiers represents one row of atoms in a crystal. All the atoms are the same, so this model represents an element.

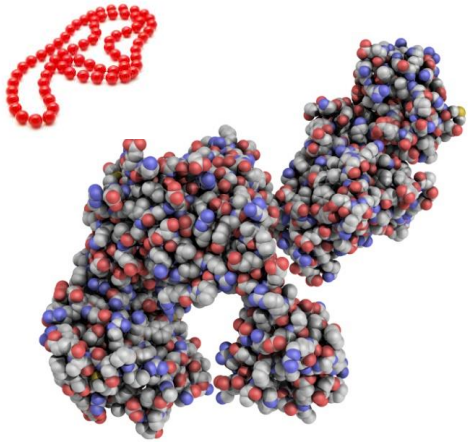
Key Stage 3 – Crystal Modelling

## Model C - fruit

Each orange represents an atom in a crystal. All the atoms are the same, so this model represents an element.

The oranges are arranged in a regular pattern.

## Model D - beads



Each bead represents one amino acid. An amino acid is a group of 10 or more atoms (including carbon, hydrogen, oxygen and nitrogen) that are strongly joined together.

You can make move the string of beads to make different patterns. A protein crystal is like a string of beads that is held in a certain pattern so that it has its own shape.

# Key Stage 3 – Crystal Modelling

## Model E - medical X-ray

Doctors use X-rays to see bones in your body. Crystallographers use X-rays to discover how atoms are arranged in crystals.

## Model F – light and cloth

Hold a piece of white cloth in front of a bright light. Stretch in out. The pattern you can see is like an X-ray diffraction pattern.

How does the pattern change if you rotate the cloth? What happens if you stretch the fabric more, or less?



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## Model G - what we cannot see

In X-ray crystallography we see things in a different way. It is a bit like trying to identify shapes in a bag with your eyes closed.

Put some items in a bag. Ask someone else to find a certain item without looking.

## Model H - what is an X-ray?

An X-ray is a wave. It transfers energy from place to place, just like waves in the sea.

X-rays carry energy at the speed of light.

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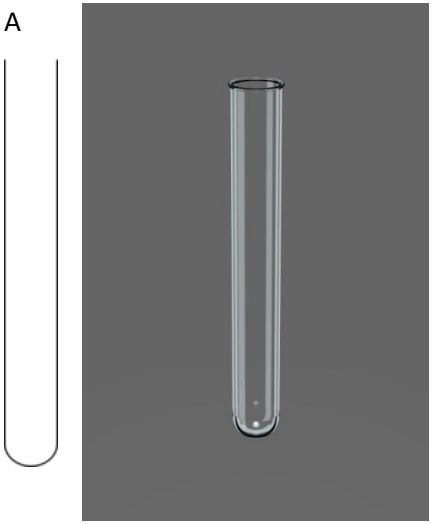
## Model I - crystal

Look at the crystal. What observations can you make about its shape?

What might your observations suggest about the arrangement of its atoms?

## Model J - 2D to 3D

A



computer program uses maths to convert many 2D images to one 3D image.

www.oxfordsparks.net/crystal

Key Stage 3 – Crystal Modelling

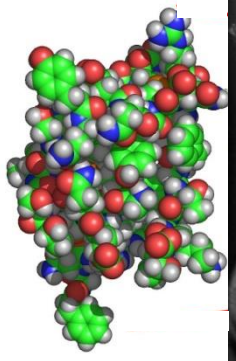
## Why is X-ray crystallography important?

Scientists use X-ray crystallography to find out how atoms are arranged in crystals. If you can obtain crystals of a substance, you can find out how its atoms are arranged.

Scientists have used X-ray crystallography to:

- Measure atoms;
- Discover the arrangement of atoms in substances such as sodium chloride (salt) and copper sulfate.;
- Work out structures of vitamins, proteins, insulin, and DNA;
- Find out how atoms are arranged in metals and minerals;
- Create new medicines ;
- Design new materials, and explain their properties.

In fact, X-ray crystallography has determined the structure of over half a million substances!



Dorothy Hodgkin used X-ray crystallography to work out the structure of insulin.

# Key Stage 3 – Crystal Modelling

## Peer assessment

The group will explain what X-ray crystallography is, how it works and why it is important. They will use models to help them explain clearly.

| Question | How clearly did they answer this question?<br>1 = not clear<br>3 = very clear |
|---|---|
| What is X-ray crystallography? | |
| How does X-ray crystallography work? | |
| Why is X-ray crystallography important? | |

1. How did the models help you understand X-ray crystallography?

2. Suggest one improvement.



Key Stage 3 – Crystal Modelling

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## Modelling help sheet

| Question | What we will say |
|---|---|
| What is X-ray crystallography? | |
| Why is X-ray crystallography important? | |

| How does X-ray crystallography work? | Models that help to explain this stage | What we will say |
|---|---|---|
| Stage 1 | | |
| Stage 2 | | |
| Stage 3 | | |
| Stage 4 | | |
| Stage 5 | | |