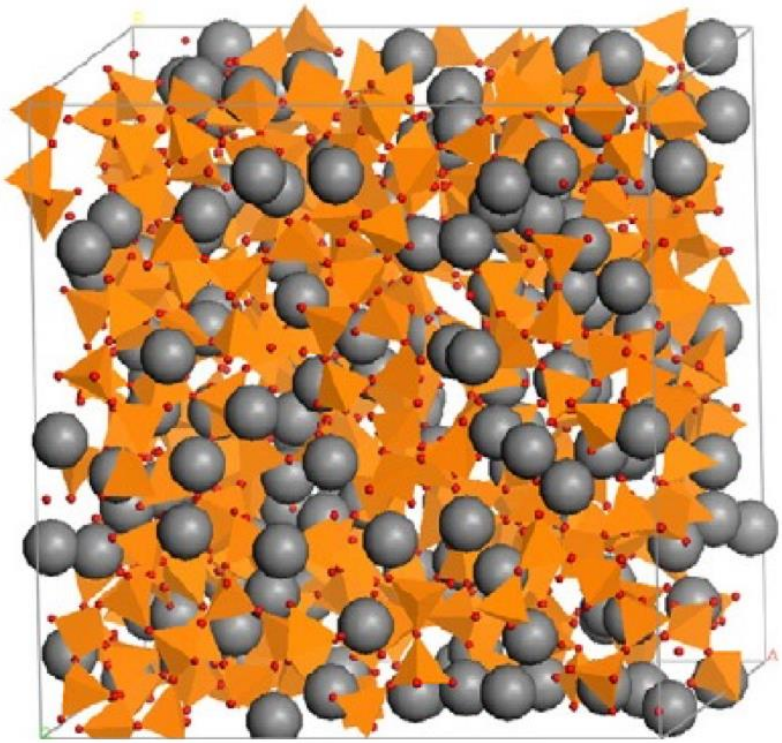
Researchers in Schools



Modelling the atomic structure of glass

Key Stage 4 Programme

Pupil Name	
Coursebook Designed by	Dr Maha Rai

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Uni Pathways launch event

Welcome to Uni Pathways! We are delighted to be able to launch the Uni Pathways programme with you. We hope that you are ready to embark on your Uni Pathways journey and that you enjoy the video.
You will be asked to pause the video at times to complete some work in this workbook, so make sure you have a pen / pencil to hand when you start the video.

By the end of the video, you will have

- Learnt about what studying at university means
- Learnt about some of the skills that you will develop during Uni Pathways
- Heard from pupils who have participated in Uni Pathways or The Scholars Programme (which is the same programme!)
- Heard from current university students talking about what life is like at university

If you are in school your teacher will play the video. If you are at home and logged in to a session with your teacher, your teacher will play the video and show it to you. If you are participating independently your teacher will email you the link to the video or the video file. There are opportunities for you to answer some questions, and you will be told when to pause the video to answer them.

Introduction to Uni Pathways

1. Write down what you think a supra-activity is

_____
_____
_____
_____

2. Independent learning is _____
_____
_____
_____

3. Write down in your own words what resilience means, and come up with a different example to the one mentioned in the PowerPoint.

_____
_____
_____
_____
_____

4. Why do you think analysis and evaluation skills are useful in your academic career? _____

_____

_____

_____

_____

_____

5. Why do you think analysis and evaluation skills are useful in life in general? _____

_____

_____

_____

_____

_____

6. What are the different types of learning that university students do?

_____

_____

_____

_____

_____

Pupils' experience of Uni Pathways

You will now watch some pupils talk about their experience of learning a PhD topic and producing a final assignment. Some may refer to The Scholars Programme rather than Uni Pathways. As you heard in the introduction PowerPoint, The Scholars Programme is a very similar programme to Uni Pathways. Listen carefully and then respond to the questions below. Be prepared to share some of your responses with your peers.

1. How did the pupils describe talking about writing a long essay for their final assignment?

_____

_____

_____

_____

_____

2. Write down something that one of the pupils mentioned was particularly interesting in their course.

_____

_____

_____

_____

3. What were some challenges that the pupils met?

_____

_____

_____

_____

_____

Virtual campus tours

You will now go on a virtual tour of some universities! Once you have seen some of the university campuses, respond to the questions below.

1. Note down something that you liked out of any of the campus tours you saw. It may be a particular building, space, city etc.

_____
_____
_____
_____
_____
_____

2. Were there any similarities between the different university campuses? If so, what are the similarities?

_____
_____
_____
_____
_____
_____

3. If you had to pick one of those universities to go and visit in person, which one would it be and why?

_____
_____
_____
_____
_____
_____

4. Note down some of the societies that you could join at different universities

_____
_____
_____
_____
_____
_____

Meet university students!

You are about to virtually meet or hear from some current university students. If you are virtually meeting them, think about what questions you would like to ask the students, share your questions with a partner and note those questions down in the space below.

If you are not meeting them but watching some videos that they have made, use the space below to note down what else you would like to find out about university. You can then ask your teacher during Uni Pathways tutorials!

Reflection

Congratulations on completing the launch of the Uni Pathways programme. Before you go, take some time to reflect on what you have learnt by answering the following questions:

a. Are there any aspects of university style learning that you would look forward to? If so, what are they?

b. What challenges do you think students face when learning at university? How would you try to overcome these challenges?

c. What skills do you hope to develop during your Uni Pathways course?

d. What part of Uni Pathways seems the most challenging for you?

e. What are you most looking forward to about Uni Pathways?

Timetable and Assignment Submission

Timetable – Tutorials

Tutorial	Date	Time	Location
1			
2			

3			
4			
5			
6 (Feedback)			
7 (Feedback)			

Timetable – Homework Assignments

Homework Assignment	Description	Due Date
Tutorial 1		
Tutorial 2		
Tutorial 3		
Tutorial 4		
Tutorial 5		

Assignment Submission – Lateness and Plagiarism

Lateness	
Submission after midnight on 9th August	10 marks deducted
Plagiarism	
Some plagiarism	10 marks deducted
Moderate plagiarism	20 marks deducted
Extreme plagiarism	Automatic fail

Course Rationale

We cannot imagine our lives without glassy materials. They are all around us and their productions are carried out on an industrial scale for a wide variety of containers, from drinking glasses to bottles to cookware. They are widespread in construction of architectural buildings, laboratories and electronic technology. Advancement of science and technology depends on the innovation of new type of glasses. Hence, it is essential that we study the atomic structure of such noble materials to understand better why they possess characters of universal engineering materials and discover new type of glasses for the future uses.

In this course we will learn to describe the structure of glasses and crystals in term of their atomic structure. We will use the simple idea of a particle model from Key Stage 3 to understand how intermolecular forces determine the positions of individual atoms and which in turn, dictates the chemical structure of a material. The chemical structure includes the type of bonds, bond angles, the size of the molecule and the interactions between molecules. Finally, the course will complete by understanding how the physical properties of glasses are due to its chemical structure.

This course will provide students with how to reduce the complexity of atomic structure into a simple ball and stick model to describe the chemical structure of complex materials like glass. The students will appreciate that the Newton's motion of equation not only describes the motion of mechanical objects we see around, but also the forces acting between the atoms and molecules. Finally, the pupil will develop analytical skills by writing an academic essay evaluating graphical and tabular results and referencing their sources.

Uni Pathways Mark Scheme 2021 – science-based assignments

	Subject Knowledge	Critical Thinking	Written Communication
1st	The work shows a depth of knowledge and understanding of key concepts and scientific methods, through engaging with relevant sources. Knowledge is used to build and support highly effective scientific arguments and explanations.	Analyses key scientific evidence, arguments, and reasoning. Interprets meaning and makes connections. Identifies and critically evaluates key scientific arguments and evidence, deciding on their credibility, strength, and relative significance, drawing convincing conclusions.	The work has a coherent flow and is well structured. The writing style is appropriate; scientific language and key scientific terms are used accurately and effectively to support the arguments and explanations made. There are no, or very few, errors in spelling or grammar. Consistent referencing, appropriate paragraphing and use of correctly labelled tables and graphs matching the style taught in the course.
2:1	The work shows an understanding of key concepts and scientific methods, drawing on relevant sources. Knowledge is used to build and support effective scientific arguments and explanations.	Analyses relevant scientific evidence, arguments, and reasoning. Identifies and critically evaluates relevant scientific arguments and evidence, deciding on their credibility and strength, drawing reasonable conclusions. Shows some understanding of the relative value of evidence and arguments.	The work is well-structured. The writing style is appropriate; scientific language and key terms are used correctly. There are few errors in spelling or grammar. Mostly consistent referencing and use of tables and figures; matching the style taught in the course.
2:2	The work shows an understanding of key concepts and scientific methods, with no major misconceptions. Beginning to apply this knowledge to build and support effective scientific arguments and explanations.	Identifies and uses basic scientific evidence, arguments, and reasoning. Showing some understanding of the quality of scientific arguments and evidence. Not yet showing understanding of the relative value of evidence and arguments.	The work has some structure. The writing style can sometimes be informal; occasionally scientific language and key terms are not used when it would be appropriate to do so. There are some errors in grammar and spelling do not get in the way of communicating the content. Referencing has some consistency; matching the style taught in the course Limited use of tables and graphs.
3rd	Shows a developing understanding of key concepts and scientific methods, with some misconceptions.	Beginning to analyse scientific evidence, arguments, and reasoning.	The grammar, spelling, style, and structure of the work need improving in order

	Does not yet apply this knowledge to build and support scientific arguments and explanations.	Describes evidence and arguments, while not yet evaluating them.	to communicate ideas to the reader. Scientific language, key terms and references are not always used correctly. Limited, or no use of tables and graphs.

Baseline Assignment (essay based): Pupil Feedback Report

Name of Pupil	
Name of School	
Name of RIS teacher	
Title of Assignment	

How your assignment is graded:

Grade	Marks	What this means
1st	70+	Performing to an excellent standard at A-level
2:1	60-69	Performing to a good standard at A-level
2:2	50-59	Performing to an excellent standard at GCSE
3rd	40-49	Performing to a good standard at GCSE
Working towards a pass	0-39	Performing below a good standard at GCSE
Did not submit	DNS	No assignment received by The Brilliant Club

Lateness	
Any lateness	10 marks deducted
Plagiarism	
Some plagiarism	10 marks deducted
Moderate plagiarism	20 marks deducted
Extreme plagiarism	Automatic fail

Marks

OVERALL MARK / 100		FINAL MARK / 100 (including any deductions)	
DEDUCTED MARKS		FINAL GRADE	

If marks have been deducted (e.g. late submission, plagiarism) the teacher should give an explanation in this section:

Mark Breakdown and Feedback

Subject knowledge	
	mark
Critical thinking	
	mark
Written communication	
	mark

Final Assignment (essay based): Pupil Feedback Report

Name of Pupil	
Name of School	
Name of RIS teacher	
Title of Assignment	

How your assignment is graded:

Grade	Marks	What this means
1st	70+	Performing to an excellent standard at A-level
2:1	60-69	Performing to a good standard at A-level
2:2	50-59	Performing to an excellent standard at GCSE
3rd	40-49	Performing to a good standard at GCSE
Working towards a pass	0-39	Performing below a good standard at GCSE
Did not submit	DNS	No assignment received by The Brilliant Club

Lateness	
Any lateness	10 marks deducted
Plagiarism	
Some plagiarism	10 marks deducted
Moderate plagiarism	20 marks deducted
Extreme plagiarism	Automatic fail

Marks

OVERALL MARK / 100		FINAL MARK / 100 (including any deductions)	
DEDUCTED MARKS		FINAL GRADE	

If marks have been deducted (e.g. late submission, plagiarism) the teacher should give an explanation in this section:

Mark Breakdown and Feedback

Subject knowledge	
	mark
Critical thinking	
	mark
Written communication	
	mark

Subject Vocabulary

Word	Definition	In a sentence
Atom	The smallest part of an element that can exist. It consists of a small dense nucleus of protons and neutrons surrounded by moving electrons.	
Ion	An atom or group of atoms that has either lost one or more electrons, making it positively charged (a cation) or gained one or more electrons, making it negatively charged (an anion).	
Molecule	A molecule consists of a group of atoms that are chemically bonded together.	
Chemical reaction	A process in which two elements are mixed to form a new substance, e.g., Hydrogen atom can react with Chlorine atom to form Hydrochloric acid.	
Crystal	A solid material with a regular polyhedral shape formed by a regular arrangement of atoms. E.g., salt.	
Non crystalline	A solid material formed by an irregular arrangement of atoms in a long-range order. E.g., glass.	
Short-range order	Short-range order is the local structure of arrangement of atoms formed around shortest distance. E.g., glass atomic structure.	
Long-range order	Long-range order is the periodic structure of arrangement of atoms over long distance in a crystal.	
Interatomic potential	It describes the interaction between a pair of atoms or the interaction of an atom with a group of atoms that binds together to form a material.	
Network former	An atom (cation) that form basic buildings block of the structure of glass.	
Network modifier	An atom (cation) that modify the network structure formed by network former cation.	

Pair distribution function	Mathematical function (graph) that shows the probability to find another atom at a certain distance from a central atom (network former cation).	
Coordination number	The number of neighbouring atoms (anions, e.g., oxygen atom) hold by central atom (network former cation) in glass.	
X-ray diffraction	The technique to study the atomic structure of materials like glass or crystal by irradiating beam of x-ray on the sample that will produce diffraction patterns.	
Melt-quenching	The melt quenching technique is the traditional technique of glass making and includes mixing of ingredients (batch), heating up to a temperature higher than 1300 °C and rapidly cooling the glass melt to obtain a solid glass.	

Tutorial 1 – Why study glasses?

Tutorial Objectives

- Describe the types of solid materials; crystalline and amorphous
- Explain order and disorder of atomic structure using the particle model of atoms
- Describe short-range and long-range order structure in glasses and crystals

Starter

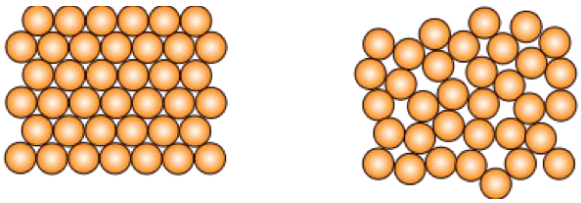
List all the application of glasses that you can think of, with their properties.

Activity 1

Draw and describe the Particle Model of Solid, Liquid and Gas.

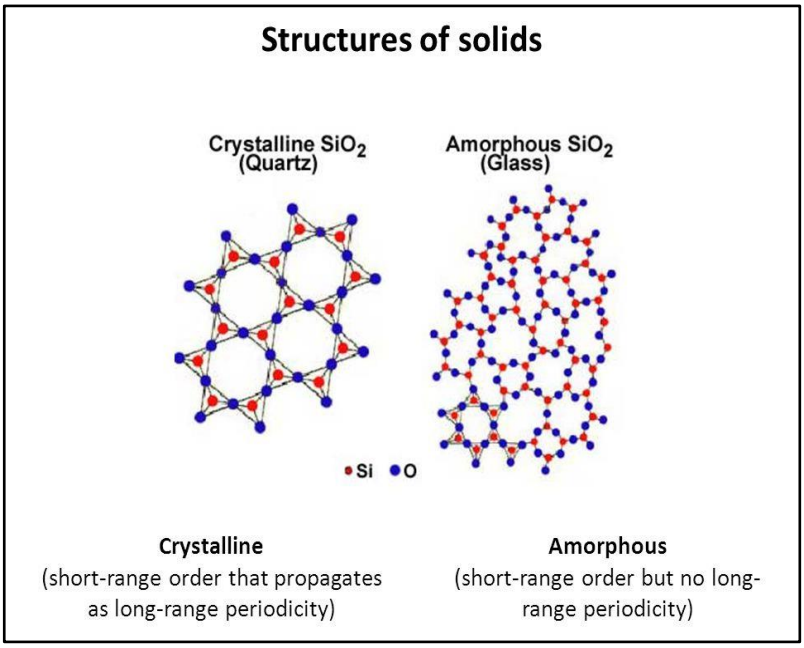
Activity 2

Explain crystalline and non-crystalline materials in terms of their atomic structure.



Activity 3

Describe short-range and long-range order structure in glasses and crystals that are made of the same base SiO_2.



Baseline Assignment **Baseline assignment instructions:**

Write an essay (500 words) about the importance of studying the structure of glasses for our everyday lives:

- Define a glass and a crystal in terms of their atomic structure
- Explain the difference between crystalline materials and glassy materials
- Describe how glasses are made by melt quenching process
- Give the essential applications of glassy materials presenting the advantages and disadvantages
- Explain how the innovation of new type of glasses advances science and technology

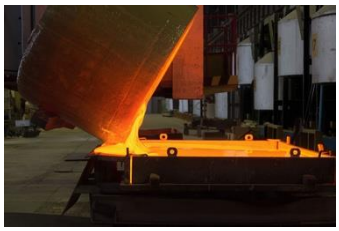
Write Baseline assignment success criteria:

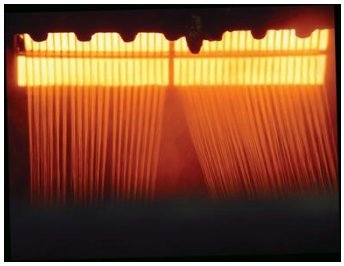
a. Include relevant content, following the examples approached in tutorial 1
b. Use appropriate scientific vocabulary from the glossary
c. Include material from a wide range of sources
d. Provide a coherent structure to your arguments
e. Include critique
f. Give reasons and evidence to back up the points. Consider using the PEE structure (point, evidence, explanation).
g. Ensure correct spelling, grammar, and punctuation
h. Make use of graphs
i. Include an introduction that informs the intention of the assignment
j. Include a conclusion that reviews the main facts and ideas
k. Reference your sources clearly
l. Write in a formal style suitable for an academic essay

Additional task not included in the baseline assignment however, it will facilitate the subsequent tutorials:

- *Revise on periodic table, Newton's Force of equation (F=ma), balanced chemical equation and slope of a graph.*

Tutorial 2 – Melt-quenching: Making of glass





Tutorial Objectives

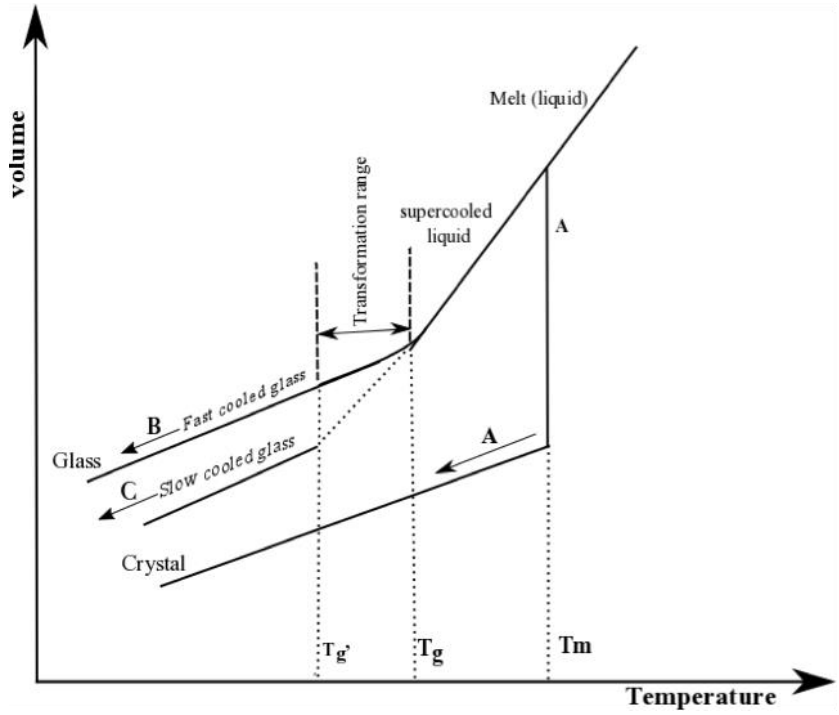
- Describe the major constituents of glass making and list all kind of glasses
- Understand the process of quenching of glass-forming substances using the volume-temperature diagram
- Describe network former and network modifier in a glass

Starter

Can you name a material that can exist as crystalline solid and non-crystalline/glassy solid?

Activity 1

Describe the process of making a glass and a crystal from the schematic diagram given below of melt-quenching.



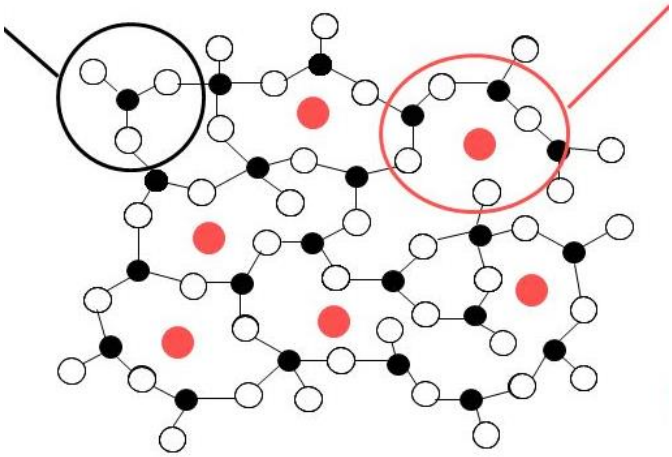
Activity 2

Name the types of glass, their properties, and applications.

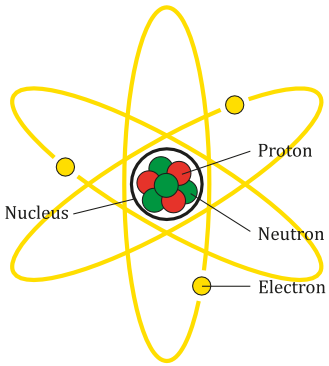
Glass Type	Properties	Applications

Activity 3

Describe network former and modifier in a glass structure.



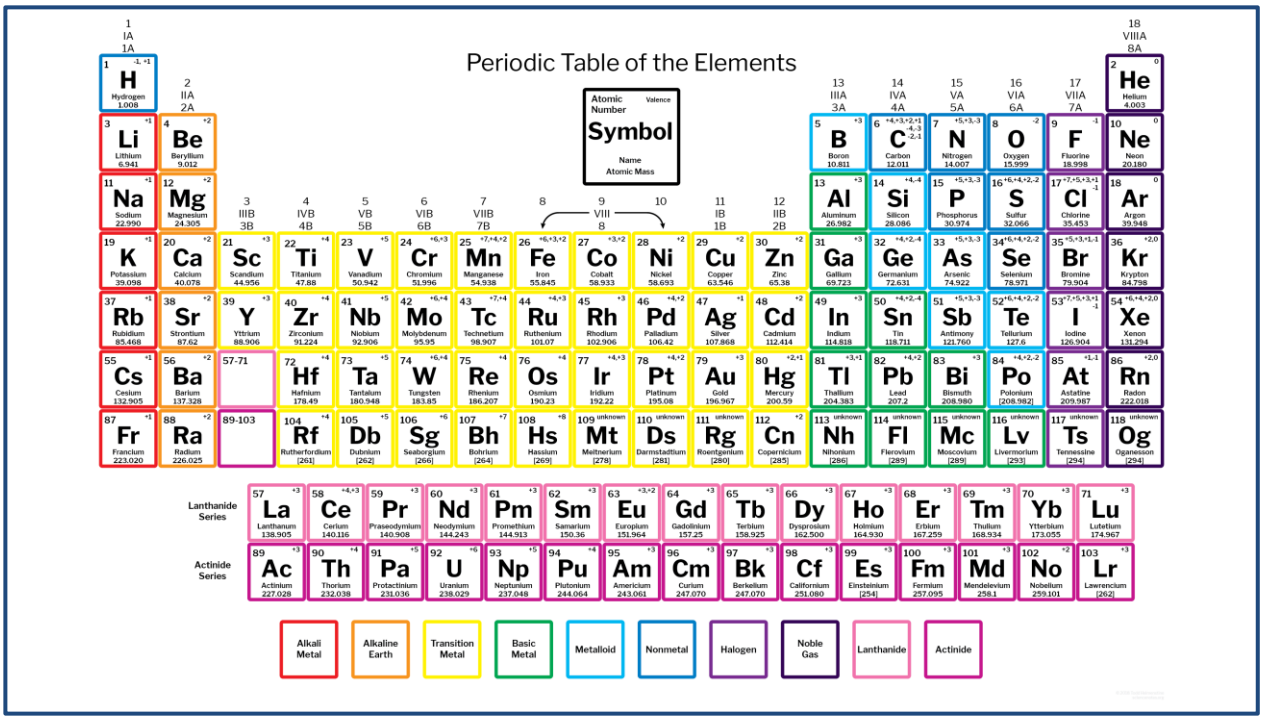
Tutorial 3 – Atoms, molecules and ions that make glasses



Tutorial Objectives

- Define an atom, element, molecule, and ion
- Describe chemical reactions that create new chemical substances
- Represent chemical reactions in terms of balance chemical equations
- Understand ionic bonding and covalent bonding in a molecule

Starter



Look up the periodic table to answer the following question:

Can you write the chemical symbol for the elements Silicon, Oxygen and Barium? Are they metal, metalloid or non-metal? Can you also write them in terms of ions?

Activity 1

How can elements make molecule?

a. Define an atom, molecule, and ion in your own words. (*hint: subject vocabulary*)
b. What is a chemical reaction?
c. Name the elements that make silica (silicon dioxide) molecule?
d. Write the balanced chemical equation for silica molecule?
e. Name the elements that make barium oxide molecule with the balanced chemical equation.

For e.g.

- *Chemical symbol for a Hydrogen element is 'H'*
- *Chemical formula for water is 'H_2O'. It constitutes of 'H' and 'O' elements.*
- *Balanced chemical equation for water is as follows:*

$$2H_2 + O_2 \rightarrow 2H_2O$$

Note: 'H' and 'O' gases exist naturally as a molecule, consisting of two atoms and are called diatomic elements.

Activity 2

Two different molecules bind together to form a crystal.

Chemical equation is the symbolic representation of a chemical reaction.

For e.g. *Magnesium dioxide reacts with silicon dioxide to form magnesium silicate. The chemical equation is as follows:*

$$MgO + SiO_2 \rightarrow MgSiO_3$$

MgO = magnesium dioxide
SiO_2 = silicon dioxide
$MgSiO_3$ = magnesium silicate

Forsterite materials consist of MgO and SiO_2 and, its chemical formula is Mg_2SiO_4. The chemical equation is as follows:

$$MgO + SiO_2 \rightarrow Mg_2SiO_4$$

The chemical equation is not balanced as there is two Magnesium atoms and four Oxygen atoms on the right-hand side whereas, there is only one Silicon atom and three Oxygen atoms on the left-hand side. Hence, the balanced chemical equation is:

$$2MgO + SiO_2 \rightarrow Mg_2SiO_4$$

The balanced chemical equation also tells us the chemical composition ratio of molecules, for e.g., there are twice the amount of MgO molecules compared to one SiO_2 molecule in Mg_2SiO_4.

a. The chemical reaction between silicon dioxide and barium oxide produces barium metasilicate. Write down the chemical equation for this chemical reaction.

b. Changing the composition ratio of barium oxide and silicon dioxide will form sanbornite **($BaSi_2O_5$)** and barium silicate **($Ba_2Si_3O_8$)**. **Balance the given chemical equations below**:

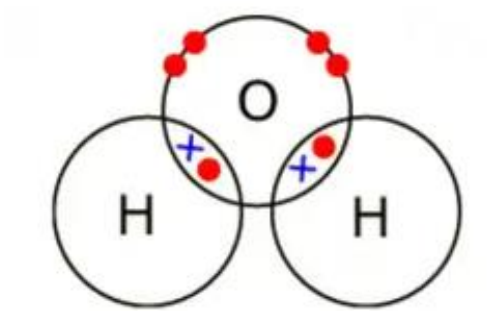
I. $BaO + SiO_2 \rightarrow BaSi_2O_5$
II. $BaO + SiO_2 \rightarrow Ba_2Si_3O_8$

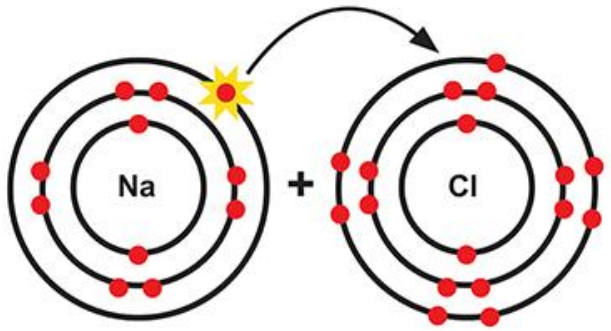
From the balanced chemical equations, write the composition ratio of barium oxide and silicon dioxide that form sanbornite **($BaSi_2O_5$)**, barium silicate **($Ba_2Si_3O_8$)** and barium metasilicate **($BaSiO_3$)**.

Activity 3

Research on Ionic bond and Covalent bond. Suggest what bonding occurs in sanbornite **($BaSi_2O_5$)** and barium metasilicate **($BaSiO_3$)** and, its constituents BaO and SiO_2.

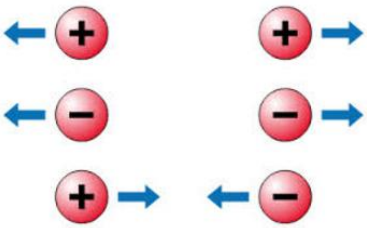
For e.g. H_2O (Water molecule) and NaCl (Salt)

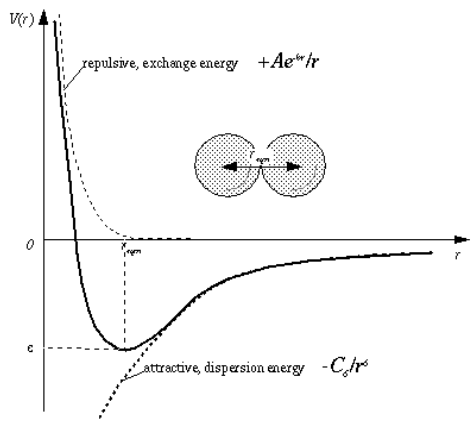




Molecule	Type of bonding
BaO	
SiO_2	
sanbornite **($BaSi_2O_5$**	
barium metasilicate **($BaSiO_3$)**	

Tutorial 4 – Interatomic potential and forces that hold glass together





The atoms and molecules in the crystal are held together by ionic forces between them.

Ionic forces are factors of:

a. *Electrostatic forces of attraction and repulsion induced by the charges present in atoms (ions)*
b. *Van der Waals attractive forces induced by electron charge cloud*
c. *Pauli repulsion forces induced by electron-electron repulsion*

Tutorial Objectives:

- Describe Electrostatic Force by Coulomb's Law
- Describe Van der Walls weakly attractive force
- Describe Pauli repulsion force

Stater

Describe the following chemical interactions between these ions.

⇒ Si – O

⇒ O – O

⇒ Ba – O

⇒ Si – Si

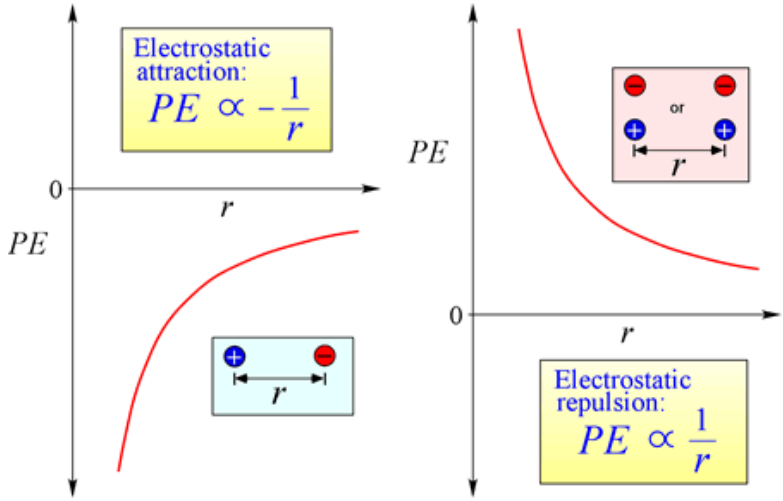
⇒ Ba – Ba

⇒ Si – Ba

Activity 1

Let's model the electrostatic forces between two ions:

*The **electrostatic force** is also known as the **Coulomb force**. It's the attractive or repulsive force between two electrically charged ions. Like charges repel each other while unlike charges attract each other.*



a. Describe the coulombic forces between two positive ions. Does the force behave the same between two negative ions?

b. Describe the electrostatic forces between a positive and a negative ion.

c. Draw the interatomic force diagram that shows the electrostatic repulsion force and electrostatic attraction force.

Activity 2

Electrostatic or Coulomb attraction force is aided by the Van der Waal force to hold together atoms in a crystal.

Negatively charged electrons orbit molecules or ions. The electrons create slightly different charges from one end of the molecule to the other. These slight differences are called partial charges, as δ^- or δ^+ which create weak attractive forces. This only takes effect when the molecules or ions are very close.

Describe Van der Waals forces in your own words.   Does Van der Waals forces contribute to the repulsion or attraction of electrostatic forces. Draw the Van der Waals force on the Interatomic force diagram?

Let's model the Pauli Repulsion force.

When two atoms, molecules or ions are attracted to each other by the electrostatic forces, the Pauli repulsion force prevents them from overlapping or coming very close together

a. Describe Pauli repulsion force in your own words.

b. Does Pauli repulsion force contribute on the repulsion or attraction of electrostatic forces. Draw Pauli repulsion force on the Interatomic force diagram?

Activity 3

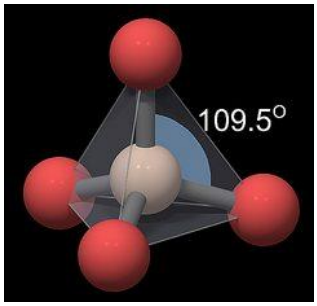
The short-range and long-range interaction of an ionic system in a two-body potential for zirconium barium fluoride system (Zr-Ba-F).

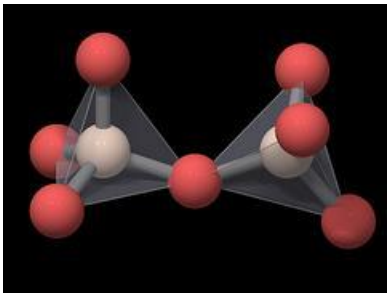
Interactions	**Electrostatic (Coulomb)** and $\propto N^2$	**Pauli Principle (Repulsive)** and $\propto N$	**Van der Walls (weakly attractive)** and $\propto N$
Equation of forces between the molecules	$(\pm)\frac{q_i q_j}{4\pi r_{ij}\varepsilon_0}$	$(+)A_{ij}\exp\left(\frac{-r_{ij}}{\rho_{ij}}\right)$	$-\frac{C_{ij}}{r_{ij}^6}$
Cation – Anion e.g. $Zr - F$ (close together)	$(-)$ Strong attraction	$(+)$ Repulsive	$(-)$weakly attractive
Anion – Anion e.g. $F - F$ (close together)	$(+)$ Repulsion	$(+)$ Repulsive	$(-)$ Weakly attractive
Cation – Cation e.g. $Zr - Zr$ (further apart)	$(+)$ Repulsion	Not applied (very weak)	Not applied (very weak)

Can you complete a similar table for Barium Silicate system (Ba-Si-O) by identifying the cations and anions.

Interactions	**Electrostatic (Coulomb)** and $\propto N^2$	**Pauli Principle (Repulsive)** and $\propto N$	**Van der Walls (weakly attractive)** and $\propto N$
Equation of forces between the molecules	$(\pm)\frac{q_i q_j}{4\pi r_{ij}\varepsilon_0}$	$(+)A_{ij}\exp\left(\frac{-r_{ij}}{\rho_{ij}}\right)$	$-\frac{C_{ij}}{r_{ij}^6}$

Tutorial 5 – Atomic structure of glasses





Silicon atoms are coloured white and oxygen atoms are coloured red. Each Silicon ion is bonded by 4 oxygen ions in a tetrahedral shape. The angle of the central O-Si-O bonds is 109.5°.

Each of the 4 oxygen atoms is linked to another silicon atom in a neighbouring tetrahedron. Silicon does not readily form double bonds to oxygen. Each oxygen atoms are shared by two tetrahedra. The Si-O-Si bond forms an angle of 144°.

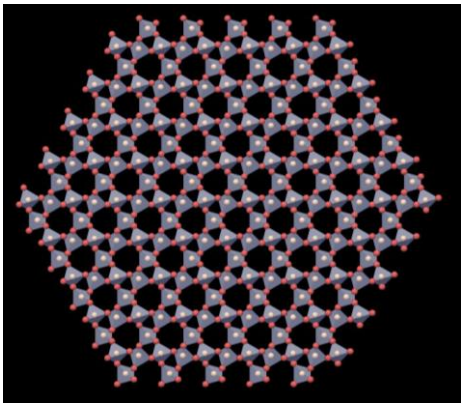
Silicon dioxide is not a 'discrete' molecule like CO_2. Silicon dioxide forms extended bonding networks containing many SiO_4 units. Quartz can thus be described as a network of interconnected SiO_4 tetrahedra.

Tutorial Objectives

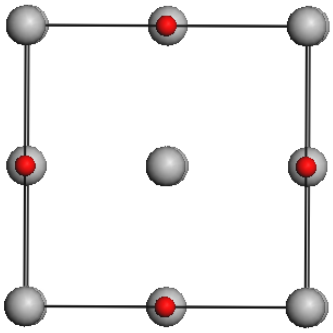
- Represent molecules in a ball and stick model and analyse the computational structure of sanbornite **($BaSi_2O_5$)** and barium metasilicate **($BaSiO_3$)** extracted from a published journal
- Describe the arrangement network formers and modifiers in a barium silicate glass, in particular sanbornite and barium metasilicate
- Describe the coordination number, bond angle and connectivity of network formers and, the validity of computer model of structure

Starter

a. Using the information above, how are SiO_4 tetrahedral structure connected in quartz? (Hint: corner sharing and edge sharing)



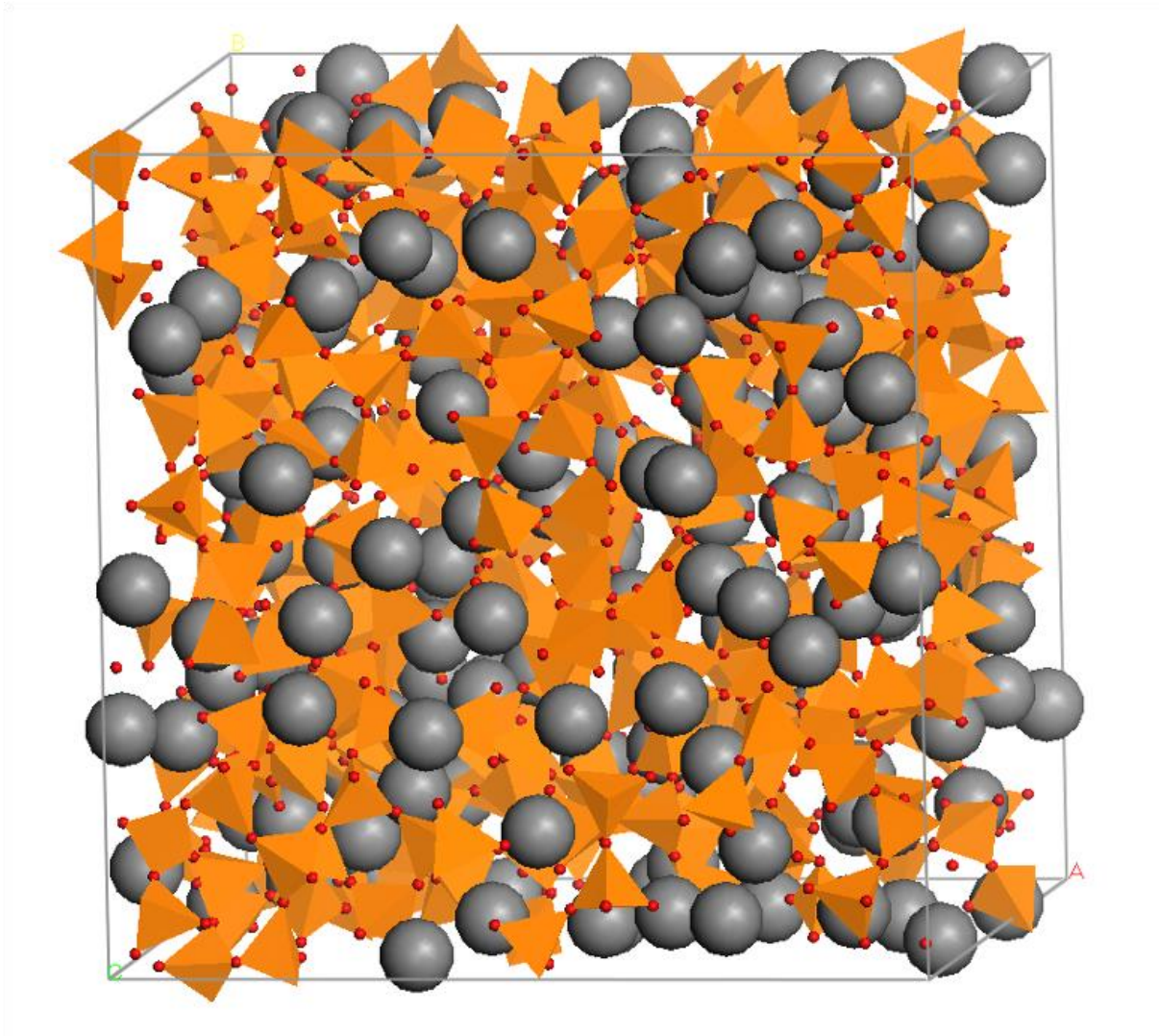
b. What is the structure of a Barium Oxide?



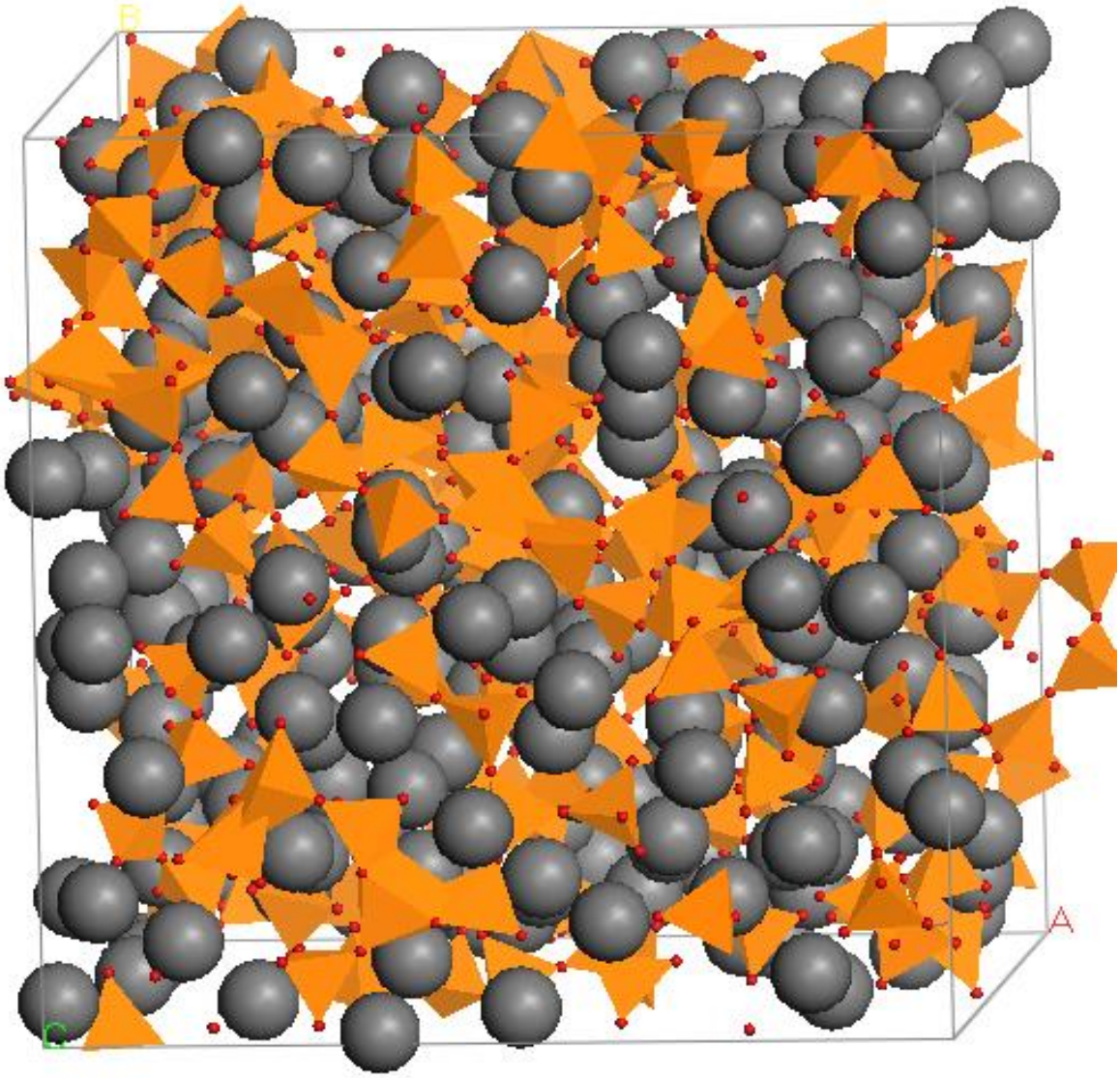
Activity 1

When molecules or atoms (represented as a sphere) join by the intermolecular forces as stated in tutorial 4, they form a structure. The following shows a computational result using molecular dynamics (Newton's equations of motion) of sanbornite and barium metasilicate, that is an extract from a Scientific Literature featured in Journal of Non-Crystalline Solids 401 (2014) 159-163.

a. Label the diagram indicating the individual atoms, network formers and modifiers in sanbornite **($BaSi_2O_5$)**. Can you tell if it is corner sharing or edge sharing?



b. Label the diagram indicating the individual atoms, network formers and modifiers in barium metasilicate **($BaSiO_3$)**. Can you tell if it is corner sharing or edge sharing?



c. Complete the table by filling the number of Barium atoms and Oxygen atoms. (Hint: Use the balanced chemical equation to find the chemical composition ratio)

Chemical compositions glasses (x)	Number of Si atoms	Number of Ba atoms	Number of O atoms	Density (gcm^{-3})	Box length (Å)	T_m (K)
Sanbornite **($BaSi_2O_5$)**	335			3.74	27.21	2000
Barium metasilicate **($BaSiO_3$)**.	240			4.21	27.21	2200

Balance the following chemical equation to determine the chemical composition ratio to help you with the above table:

I. $BaO + SiO_2 \rightarrow BaSi_2O_5$

II. $BaO + SiO_2 \rightarrow BaSiO_3$

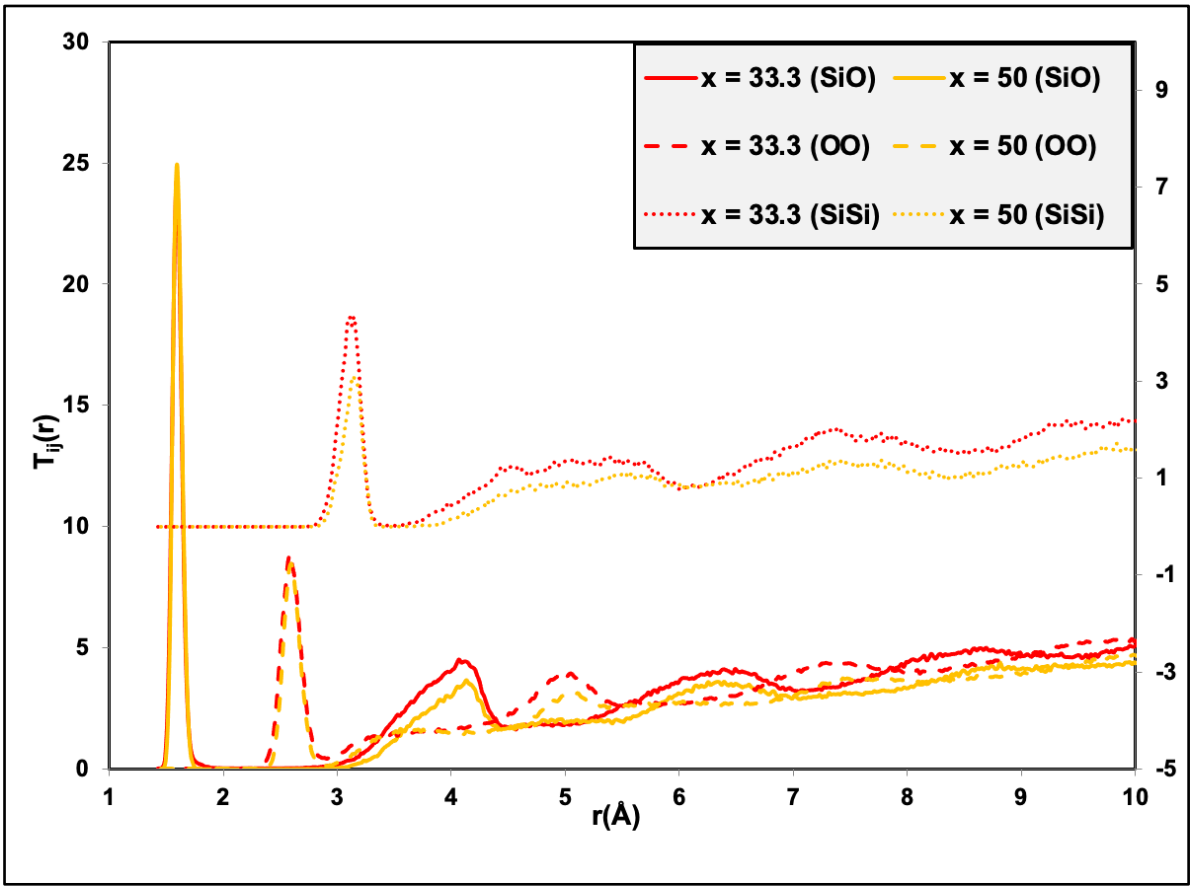
Activity 2

The graph of pair distribution function represents the probability of finding the nearest neighbours at a certain bond length. The area under the graph is the coordination number of an atom.

For e.g. In figure (a) sanbornite glass (x=33.3) the first peak in $T_{SiO}(r)$ represents Si-O nearest neighbours and is found to have a bond length of R_{SiO}=1.59 Å and coordination number N_{SiO}=4.

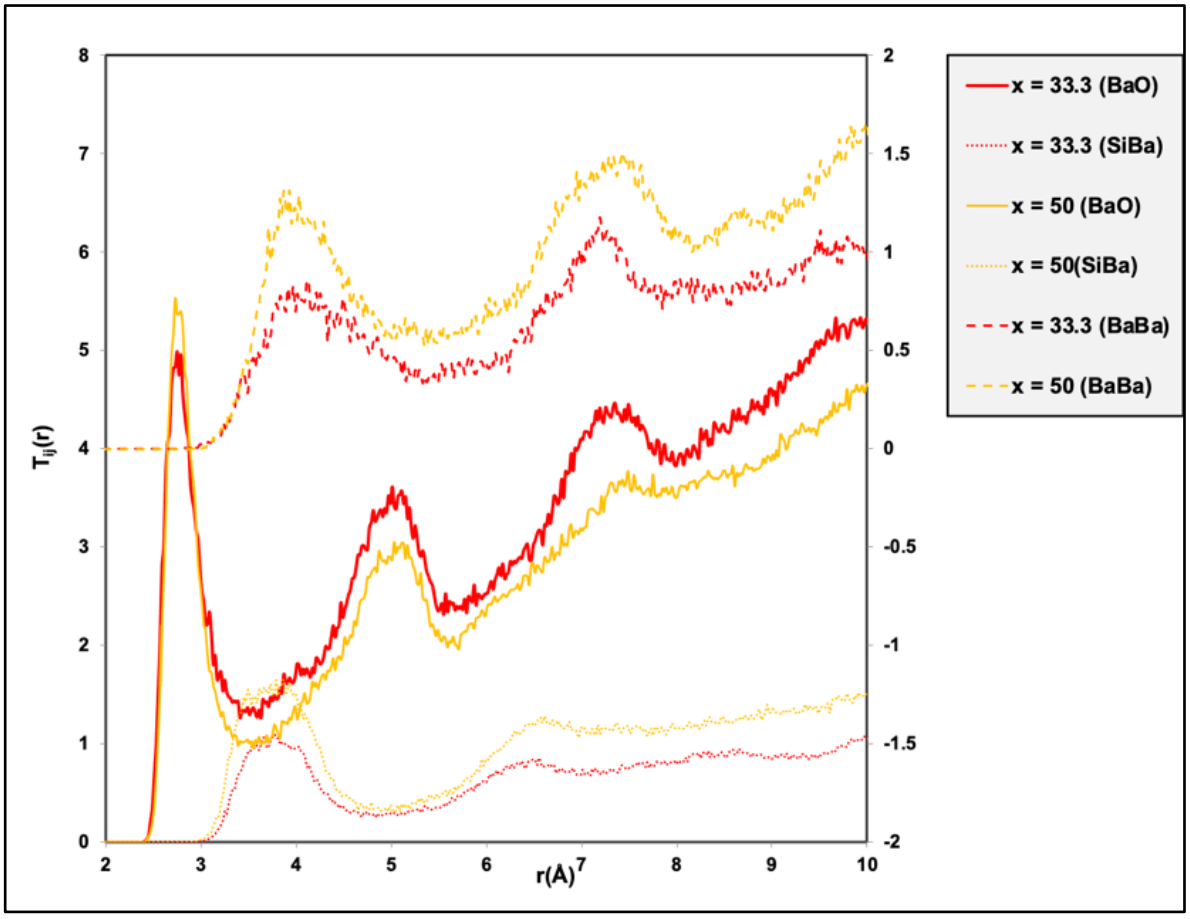
Another e.g. In figure (b) the first peak in $T_{BaO}(r)$ represents Ba-O nearest neighbours with roughly a constant Ba-O bond length R_{BaO}=2.79 Å and coordination number N_{BaO}=6.8

a. With the information above and the result provided below, could you write the coordination number (CN) and bond length of Si-O, for barium metasilicate glass (x=50) in the given table below:



Glass	Si-O R(Å)	Si-O CN
X = 33 (BS2)	1.59	4.0
X = 50 (BS)		

b. With the information above and the result provided below, could you write the coordination number (CN) and bond length of Ba-O, for barium metasilicate glass (x=50) in the given table below:



Glass	Ba-O R(Å)	Ba-O CN	Si-Si CN
X = 33 (BS2)	2.79	6.9	3.07
X = 50 (BS)			2.03

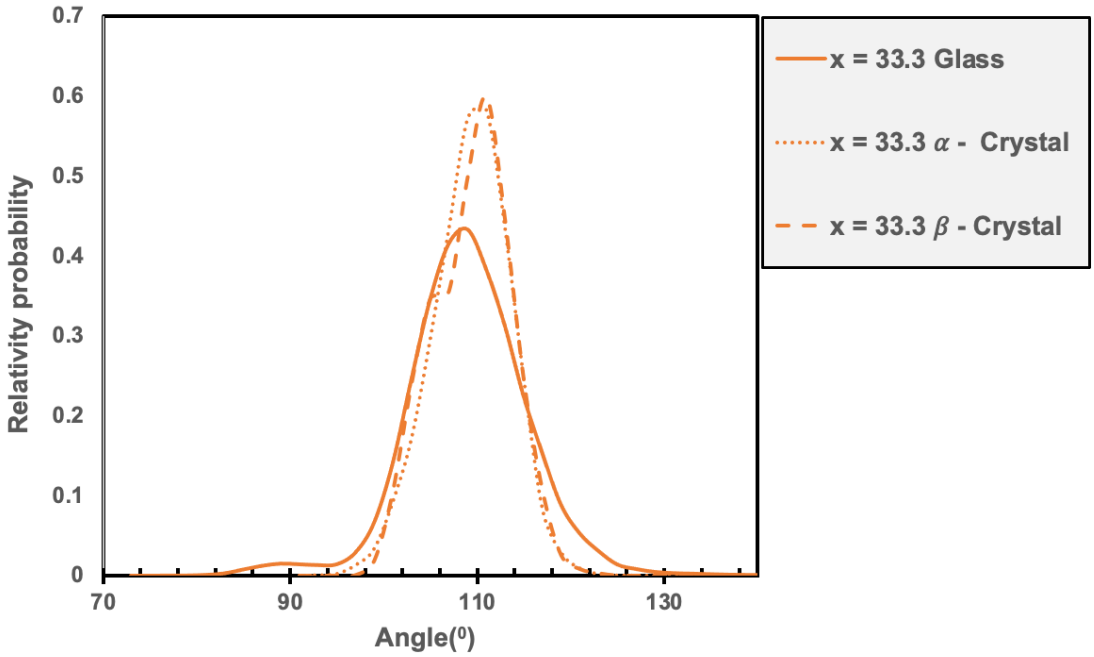
c. Si-Si in the table is the connectivity of one SiO_2 to another SiO_2 in the structure. Look carefully in the given modelled pictures in Activity 1 and comment on the Si-Si CN results.

Activity 3

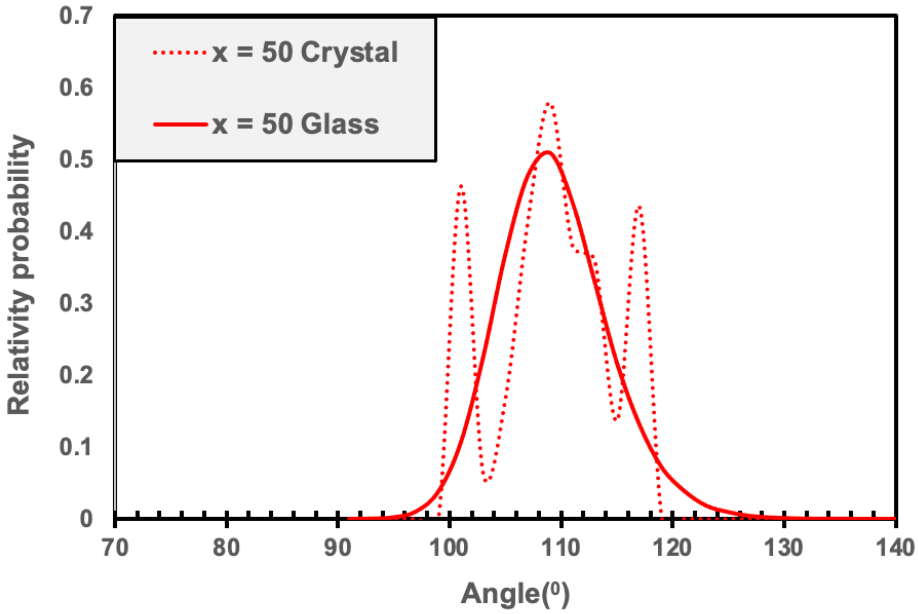
In an amorphous material, the bond angle distribution functions (BAD) describe the randomness in the structure. If we consider the atom types i and j then the bond angle, θ is the angle subtended between atoms $i - j - i$, j being the central atom type and hence, the inter-connections between atoms inside the structural units can be analysed in term of BAD.

The figure below shows the BAD subtended by two oxygen, O, atoms at silicon, Si, atoms i.e., $O - Si - O$. The crystalline structure will have a narrow distribution centred on a single value however, the amorphous will have a broad angle distribution due to the static variation, structural and thermal disorder.

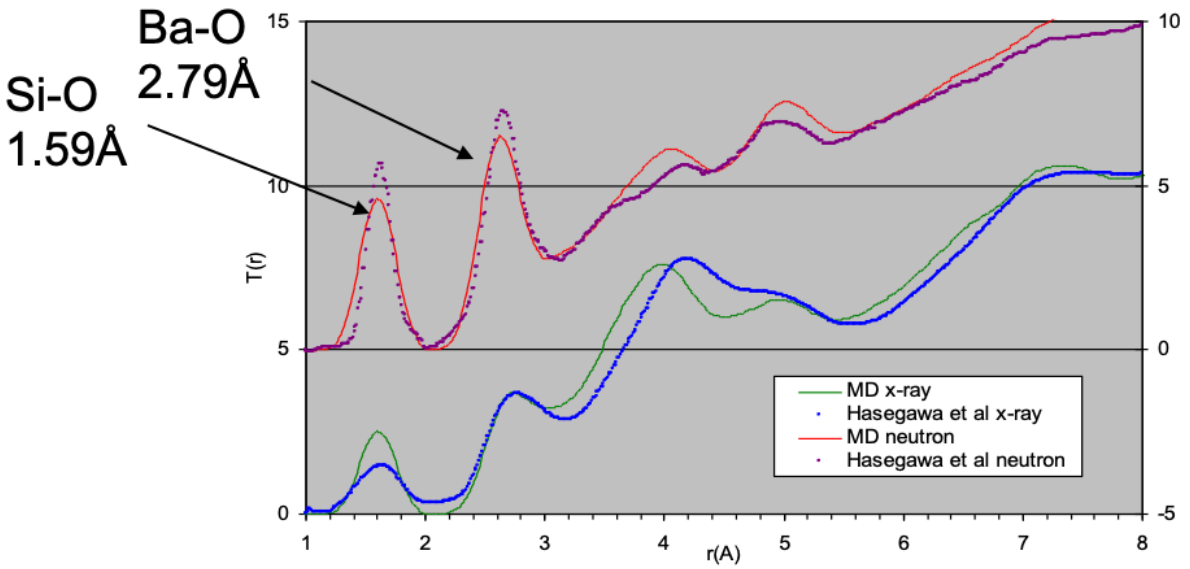
a. From the figure below suggest the values of BAD on sanbornite glass and crystal.



b. Calculate the BAD for barium metasilicate glass and crystal (x=50) from the given below graph. Find all the three peaks of x=50 crystals and describe the structure of this tetrahedra.



The model structure is always validated with the experimental results. Below shows the comparison of pair distribution function mentioned in Activity 2 calculated from the computer model, compared with the experimental result obtained from the X-ray and neutron diffraction for sanbornite glass.



Pair distribution function T(r) from neutron and x-ray diffraction

I. Comment on the validity of the sanbornite presented above.

II. What do scientist need to do to validate the computer model of barium metasilicate glass (x=50).

Final Assignment

Write a 2000 words essay detailing all the key concepts learned throughout the activities. Your report should focus on SiO_2 glass and barium silicate glasses and, the following:

- Structure of glasses and crystals in term of their atomic structure
- Particle model to understand how intermolecular forces determine the positions of individual atoms
- The chemical structure including the type of bonds, bond angles, the size of the molecule and the interactions between molecules
- How the physical properties of glasses are influenced by its chemical structure
- Representing molecules in a ball and stick model and analysing the computational structure
- The coordination number, bond angle and connectivity of network formers and, the validity of computer model of structure

You can use your Baseline Assignment to introduce your essay. (Hint: you are encouraged to use each tutorial objectives as a guideline to your essay)

Success criteria:

- Demonstrate knowledge and understanding specified in the assignment.
- Use technical vocabulary from the glossary and elsewhere appropriately.
- Include research from a variety of sources.
- Give reasons and evidence to support your analysis and conclusions. Consider using the PEE structure (point, evidence, explanation).
- Organise your work in paragraphs, with a logical structure. Using section headings as described above. Include an introduction that outlines the topics your assignment covers. Include a conclusion that refers to your analysis and evaluation.
- Analyse your data correctly and accurately and use your evaluation of the data to support your conclusions.
- Make sure your spelling, grammar, punctuation and use of scientific notation are accurate.
- Reference your sources clearly.
- Write in a formal style suitable for an academic essay.

Tutorial 6 – Feedback tutorial

What is the Purpose of Tutorial 6?

- To receive feedback on your final assignment
- To respond to the feedback from your Uni Pathways teacher
- To write targets for improvement on your final assignment

Final assignment feedback from your Uni Pathways Teacher

(Remember to look at the mark scheme to help you understand what you have done well so far, and how you can do even better in your final assignment)

Here are three things that my Uni Pathways Teacher thought I did well in my draft assignment
•   •   •

Here are three things that my Uni Pathways Teacher thinks that I could do to get a higher mark in my final assignment
•   •

•

Tasks from my Uni Pathways Teacher to do during the feedback tutorial to help me improve
•   •   •
My response:

Actions I will take to improve my final assignment after this tutorial…
•   •   •

Hand in date for my final assignment:	

Tutorial 7 – Final tutorial

What is the Purpose of Tutorial 7?

- To receive feedback and a grade on your final assignment.
- To reflect on the programme including what you enjoyed and what was challenging.
- To ask any questions you may have about university.

Final assignment feedback from my Uni Pathways Teacher

Final mark:	University style grade:
Feedback: Here are three things that my Uni Pathways teacher thought I did well in my final assignment • • •	

Here are three things that my Uni Pathways teacher thinks I should remember for when I am doing this kind of study in the future
• • •

University

What questions do you still have about University after taking part in Uni Pathways?
● ● ●

Reflecting on Uni Pathways

What did you most enjoy about Uni Pathways?
● ● ●

What did you find challenging about the programme?	How did you overcome these challenges?
● ● ●	● ● ●

Appendix 1 – Referencing correctly

When you get to university, you will need to include references in the assignments that you write, so we would like you to start getting into the habit of referencing in your Brilliant Club assignment. This is really important, because it will help you to avoid plagiarism. Plagiarism is when you take someone else's work or ideas and pass them off as your own. Whether plagiarism is deliberate or accidental, the consequences can be severe. In order to avoid losing marks in your final assignment, or even failing, you must be careful to reference your sources correctly.

What is a reference?

A reference is just a note in your assignment which says if you have referred to or been influenced by another source such as book, website or article. For example, if you use the internet to research a particular subject, and you want to include a specific piece of information from this website, you will need to reference it.

Why should I reference?

Referencing is important in your work for the following reasons:

- It gives credit to the authors of any sources you have referred to or been influenced by.
- It supports the arguments you make in your assignments.
- It demonstrates the variety of sources you have used.
- It helps to prevent you losing marks, or failing, due to plagiarism.

When should you use a reference?

You should use a reference when you:

- Quote directly from another source.
- Summarise or rephrase another piece of work.
- Include a specific statistic or fact from a source.

How do I reference?

There are a number of different ways of referencing, and these often vary depending on what subject you are studying. The most important to thing is to be consistent. This means that you need to stick to the same system throughout your whole assignment. Here is a basic system of referencing that you can use, which consists of the following two parts:

1. **A marker in your assignment**: After you have used a reference in your assignment (you have read something and included it in your work as a quote, or re-written it your own words) you should mark this is in your text with a number, e.g. [1]. The next time you use a reference you should use the next number, e.g. [2].
2. **Bibliography**: This is just a list of the references you have used in your assignment. In the bibliography, you list your references by the numbers you have used, and include as much information as you have about the reference. The list below gives what should be included for different sources.

    a. **Websites** – Author (if possible), title of the web page, website address, [date you accessed it, in square brackets].

    E.g. Dan Snow, 'How did so many soldiers survive the trenches?', http://www.bbc.co.uk/guides/z3kgjxs#zg2dtfr [11 July 2014].

    b. **Books** – Author, date published, title of book (in italics), pages where the information came from.

    E.g. S. Dubner and S. Levitt, (2006) *Freakonomics*, 7-9.

    c. **Articles** – Author, 'title of the article' (with quotation marks), *where the article comes from* (newspaper, journal etc.), date of the article.

    E.g. Maev Kennedy, 'The lights to go out across the UK to mark First World War's centenary', Guardian, 10 July 2014.

Notes

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