Experiment No:02

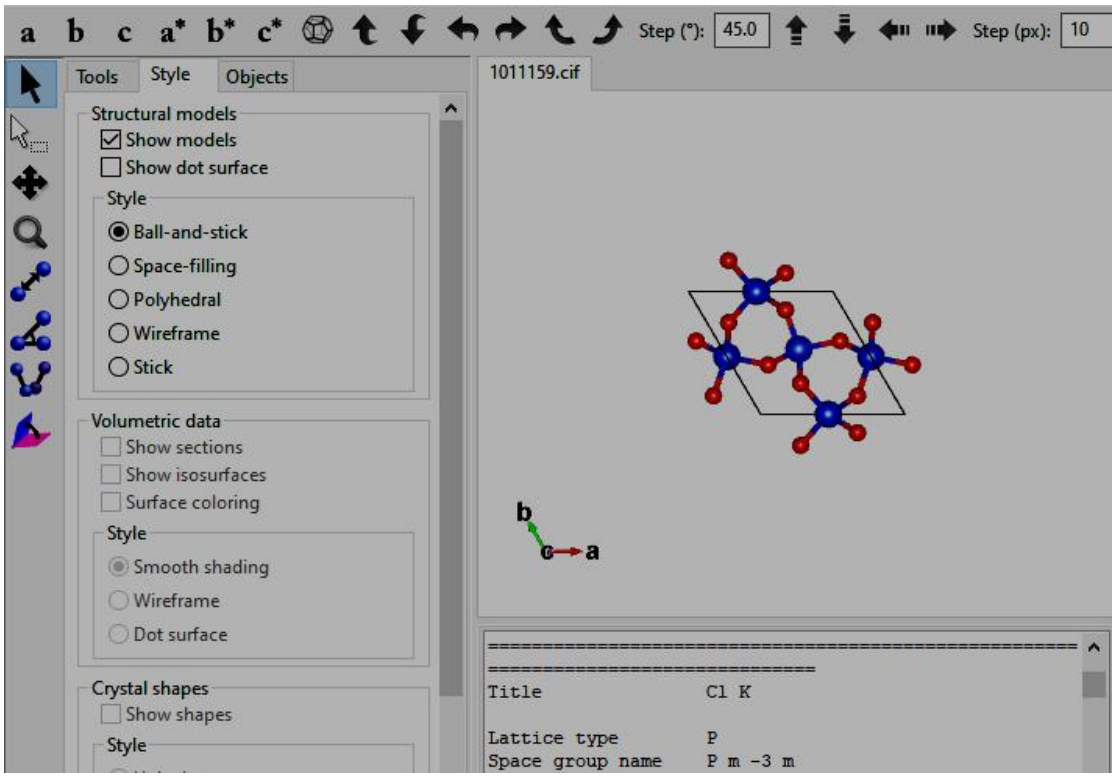
To contract and visualize unit cells of solid structures using data obtained from crystallographic information file (CIF).

Abstract:

To investigate the crystal structures of various solids by visualizing their unit cells using crystallographic information files (CIF). By importing CIF data into VESTA software, generated the different representations of unit cells, revealing insights into atomic arrangement, bonding and packing. Findings show that the unit cell exhibit diverse crystal systems, lattice parameters and space groups. Conclusions show that CIF- based unit cell visualization is a powerful tool for understanding structures and materials properties, enabling precise analysis and interpretation of crystallographic data.

Introduction:

VESTA (visualization for Electronic and Structural Analysis) is a comprehensive software tool designed for the visualization and analysis of crystallographic data. Developed by the institute for solid state physics at the university of Tokyo, VESTA provides an intuitive and user-friendly interface for researchers to explore and understand the structural properties of crystalline and molecular solids. It enables the discovery of new materials and optimization of existing one.



Title Si O2

Lattice type C
Space group name Custom
Space group number 154
Setting number 1

Lattice parameters

a	b	c	alpha	beta	gamma
4.91000	4.91000	5.40000	90.0000	90.0000	120.0000

Unit-cell volume = 112.742421 Å^3

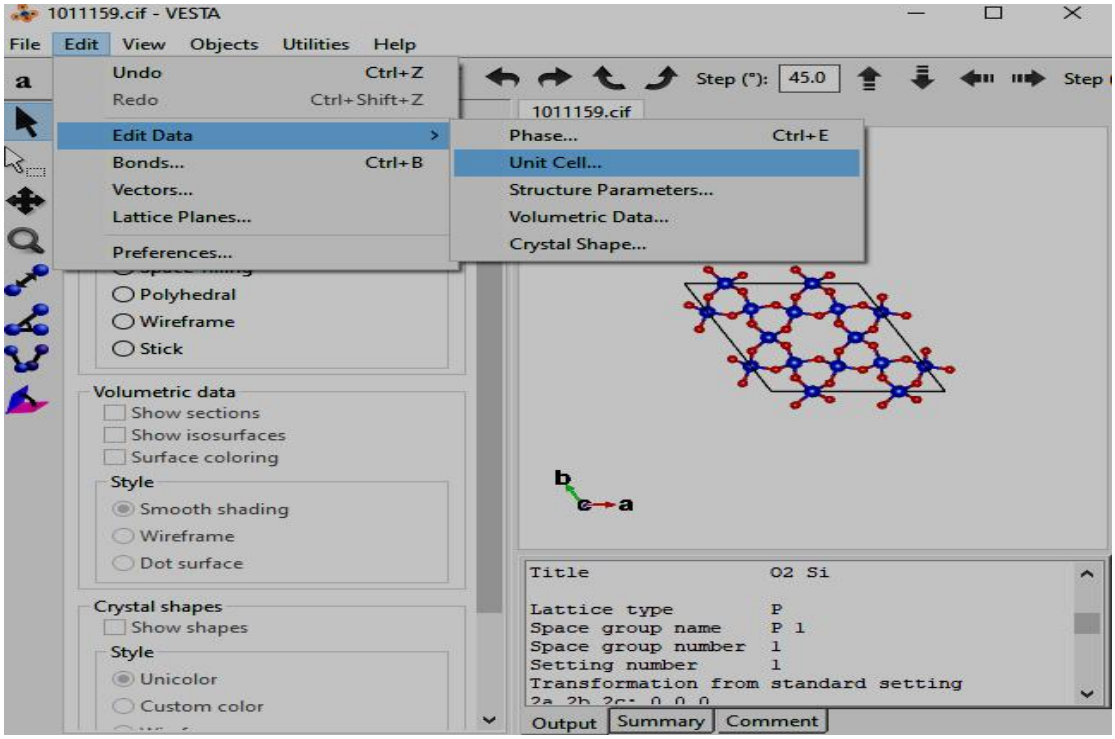
Structure parameters

			x	y	z	Occ.	U	Site	Sym.		
1	Si	Si1		0.469	0.00000	0.00000	1.000	-0.000	3		-
2	O	O1	0.40300	0.25300	0.12200	1.000	-0.000	6		-	

Number of polygons and unique vertices on iso surface = 0 (0)
29 atoms, 28 bonds, 7 polyhedral; CPU time = 1 ms
142 atoms, 152 bonds, 38 polyhedral; CPU time = 5 ms

Unit cell:

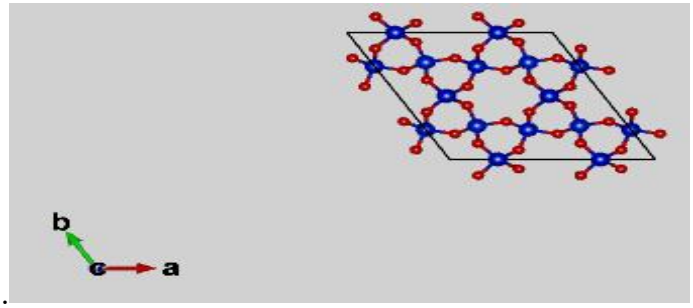
A unit cell is the smallest portion of a crystal lattice that shows the three-dimensional pattern of the entire crystal. A crystal can be thought of as the same unit cell repeated over and over in three dimensions.



Visualization of unit cell:

The unit cell is defined as the smallest repeated unit with full crystal structure symmetry. The unit cell geometry is known as a parallelepiped, providing six lattice parameters taken as the lengths of the edges of the cells (a, b , c) and the angles between them (α, β, ɣ).

Opposite faces of a unit cell are parallel.The edge of the unit cell connects equivalent points.



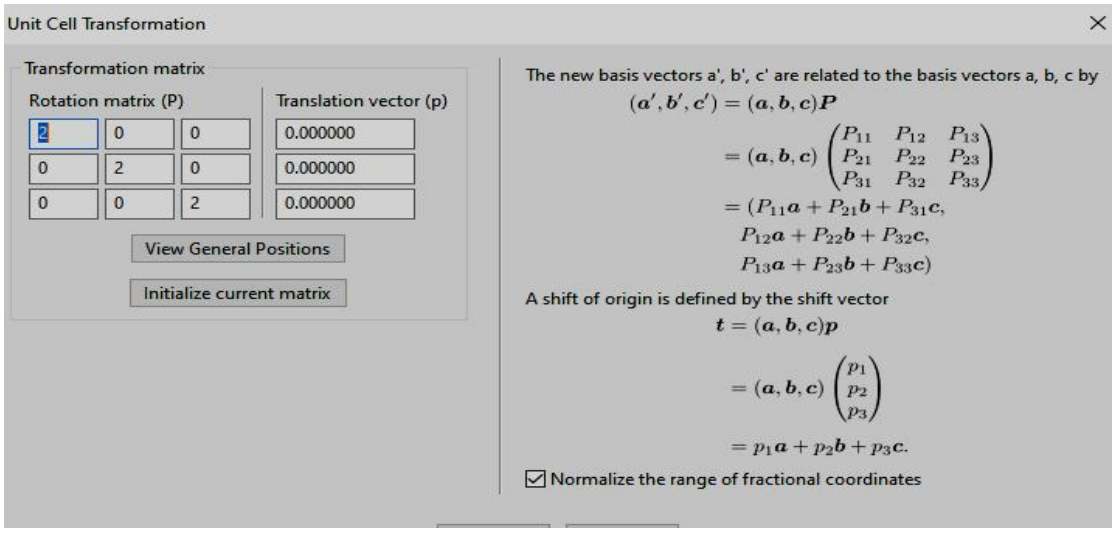
Title : SiO2
Lattice type : P
Space group name P 32 2 1
Space group number 154
Setting number 1
Transformation from standard setting 2a,2b,2c; 0,0,0
Transformation to standard setting 1/2a,1/2b,1/2c; 0,0,0

Lattice parameters

a	b	c	alpha	beta	gamma
9.82000	9.82000	10.80000	90.0000	90.0000	120.0000

Unit-cell volume = 901.939368 Å^3

Unit cell transformation:

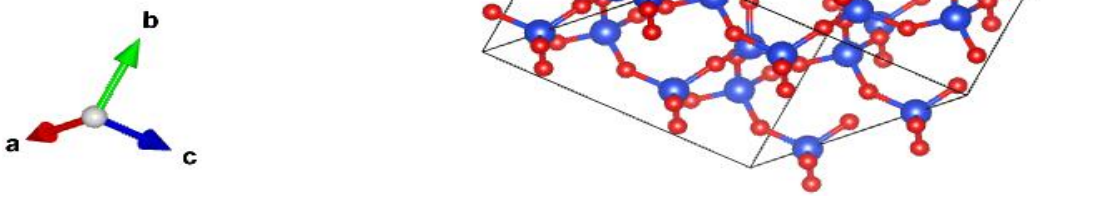


Contraction of unit cell:

Niggli - reduced cell:

A niggli- reduced cell is a standardized representation of a crystallographic unit cell, where the unit cell axes and angles are optimized to meet specific conditions.The goal is to obtain a unique and compact representation of the unit cell making it easier to:

- Comparison of crystal structures
- Identification of symmetry
- Calculation of lattice parameters and density



Reduced cell Transformation into Niggli - reduced cell

Cell parameters after reduction :
4.9100 4.9100 5.4000 90.0000 90.0000 120.0000
total transformation = -a-b,b,c

Reduced form 12 , which means metrically Hexagonal hP

Axes a and b of reduced cell are very similar.
Niggli reduced cell option; new space group: 1 P 1

Atoms in asymmetric unit of new space group :

Si	1	0.53100	0.53100	0.00000
Si	1	0.00000	0.46900	0.66667
Si	1	0.46900	0.00000	0.33333
Si	1	0.53100	0.53100	0.33333
Si	1	0.46900	0.00000	0.66667
Si	1	0.00000	0.46900	0.00000
O	1	0.59700	0.85000	0.12200
O	1	0.25300	0.40300	0.78867
O	1	0.15000	0.74700	0.45533
O	1	0.85000	0.59700	0.21133
O	1	0.40300	0.25300	0.54467

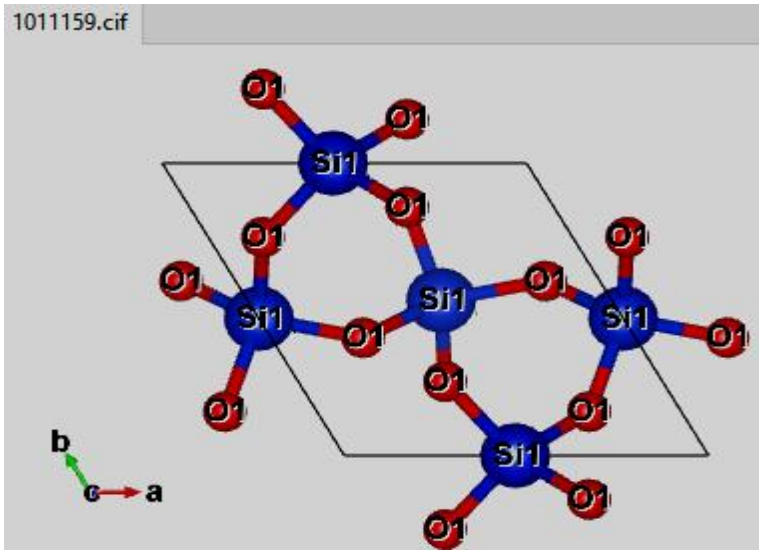
Equipment's Or Accessories:

- Compute or laptop with VESTA software installed
- Crystallographic data files (CIF)
  Silicon dioxide (SiO2)

Experimental Design:

i. I launch VESTA software and obtain a CIF file of SiO2 from online databases
ii. Then open the CIF file of SiO2 in VESTA.
iii. First I, obtain the the Unit cell of SiO2. Then I visualize this Unit cell by using VESTA software tools:
Click on Edit menu. Then click on Edit data. After this I go on unit cell tool.
In unit cell tool click on transform then , change the diagonal position.
I choose 2 position on diagonal. The apply on the structure click on OK.
Finally I obtain a unit cell.
iv Then I, visualize this unit cell by lattice type, lattice parameters(angles and bonds), structure parameters and their unit cell volume.
v Then I contract the unit cell by using utilities menu, then click on niggli- reduced cell.
vi Finally I contract the unit cell into Niggli- reduced cell , and obtain a unique and compact representation of unit cell.
Vii Then I compare the actual unit cell and Niggli- reduced cell also identify the symmetry of structures, find their lattice parameters and density.

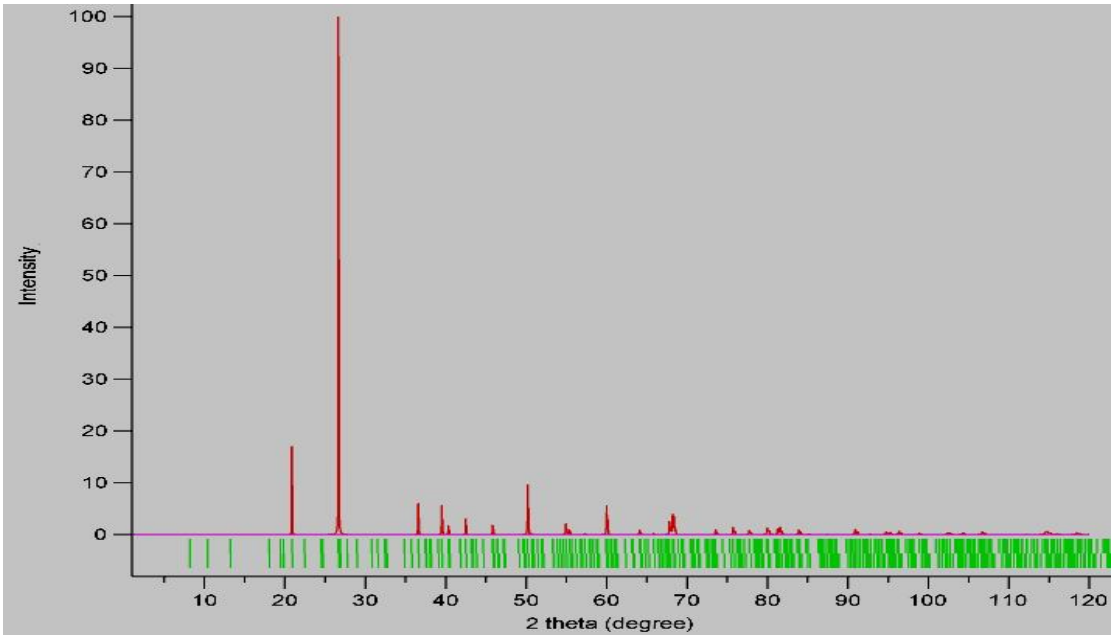
Structure:



Observations:

h	k	l	Diffraction angle(2ɵ)	Intensity (I)	Wavelength (λ)	d(A^0)
0	2	2	26.6618	100.00	1	3.34077
0	2	2	26.7276	49.7447	2	3.34077
2	0	2	26.6618	43.3426	1	3.34077
2	0	0	20.8739	22.5145	1	4.25218

Analysis:



Output:

Unit cell transformation of SiO2:
Space Group: P 32 2 1

Bond lengths:
a = 9.82000 Å
b = 9.82000 Å
c = 10.80000 Å

Bond angles:
α = 90.0000°
β = 90.0000°
γ =120.0000°

V = 901.9394 Å^3
Space group name: Custom
Transformation from standard setting 2a,2b,2c; 0,0,0
Transformation to standard setting 1/2a,1/2b,1/2c; 0,0,0

Contraction of Unit cell into Niggli- reduced cell:

Cell parameters after reduction :
4.9100 4.9100 5.4000 90.0000 90.0000 120.0000
total transformation = -a-b,b,c
new space group: 1 P 1
Reduced form 12 , which means metrically Hexagonal hP
Note: Axes a and b of reduced cell are very similar.

Conclusion:

I successfully visualized the unit cell of SiO_2 , also their contraction by using Crystallographic data from CIF file.I also visualize unit cell transformation into Niggli- reduced cell and accurate contraction of unit cells to desired sizes while maintaining crystal structure integrity. This experiment also provided effective analysis and refinement of visualized unit cells to understand solid structure properties.