Notes on Bravais lattices and Crystal Systems (Experiment 2)

(Not to be submitted)

Crystal Family	Crystal system	Characteristic Symmetry	Conventional Unit Cell Shape	Bravais Lattices
Triclinic	Triclinic	None	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$	aP
Monoclinic	Monoclinic	A single two-fold axis. (	(i) Unique axis c $a \neq b \neq c$ $\alpha = \beta = 90° \neq \gamma$	mP, mA
Orthorhombic	Orthorhombic	Three two-fold axes	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	oP, oI, oF, oC
Tetragonal	Tetragonal	A single four-fold axis	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$	tP, tI
Hexagonal	Trigonal	A single three-fold axis	(i)Rhombohedral cell $\mathrm{a} = \mathrm{b} = \mathrm{c}$ $\alpha = \beta = \gamma \neq 90°$ (ii)Hexagonal cell $a = b \neq c$ $\alpha = \beta = 90°, \gamma = 120°$	hR
			Hexagonal cell $a = b \neq c$ $\alpha = \beta = 90°, \gamma = 120°$	hP
	Hexagonal	A six-fold axis	$a = b \neq c$ $\alpha = \beta = 90°, \gamma = 120°$	hP
Cubic	Cubic	Four three-fold axes	$a = b = c$ $\alpha = \beta = \gamma = 90°$	cP, cI, cF

NOTES:

1. The symbol for Bravais lattice consists of two letters: the first small letter represents the crystal family and second capital letter represents the centring of the conventional cell Thus the first letters of the lattices of the different crystal families are:-Triclinic : a, Monoclinic : m, Orthorhombic : o, Tetragonal : t, Hexagonal : h, and Cubic : c. The letter a in the symbol for triclinic system stands for 'anorthic' meaning that no pair of the axes of the conventional cell are orthogonal. The centering symbols are: A: A-centered, B: B-centered, C: C-centred, S: (A, B, or C-centred), F: Face-centred, I: Body-centred, R: Rhombohedral centred.

2. The '$\neq$' sign should be interpreted as '*not required to be equal by the symmetry of the crystal system*'. They can sometimes be equal, these cases are known as 'accidental equality'. Equivalently '$=$' stands for 'required to be equal by symmetry of the crystal system.

3. The lattice hR of the trigonal system has two alternative conventional cells associated with it: the rhombohedral cell or the hexagonal cell. The rhombohedral cell is primitive whereas the hexagonal cell is rhombohedrally centred. This is the only lattice for which two alternative conventional cells are associated. Irrespective of the choice of the cell the lattice is called hR.

4. hP lattice belongs to both trigonal system and the hexagonal system. This is the only lattice which belongs to two different crystal systems.

APL 102: Introduction to Material Science and Engineering

Experiment 2: Two and Three-Dimensional Bravais Lattices

(A) Two-Dimensional Periodic Pattern

Crystals are nothing but three-dimensional periodic pattern of atoms. A periodic pattern can be described in terms of a lattice and a motif. We will look at some two-dimensional periodic patterns (wall papers) and identify their lattices motifs and plane groups.

A1 Lattice: An infinite set of discrete points such that each has identical neighbours of other points is called a lattice. Any point of a periodic pattern can be selected as a reference lattice point. The set of all points exactly equivalent to this point constitutes the lattice of the pattern.

i) Examine the 2D pattern of footpath tiling outside Academic Complex East.. Place a sheet of tracing paper over the pattern. Choose any point of the pattern as a reference and mark your reference point with a dot. Now mark every translationally equivalent point of the pattern with a dot. These points constitute a finite portion of the infinite lattice. [2]

ii) Keeping the edges of the tracing paper parallel to the original directions, move the paper over the pattern so that the original dot now lies above some other feature. Note that the other dots give the positions of all points in the pattern which are equivalent to the new feature. Thus, the lattice of a pattern is the same whichever initial point is chosen as a reference point. Verify the above statement for different starting positions.

A2 Unit cell: A Lattice can be described by giving its unit cell which in 2D is a parallelogram and in 3D is a parallelepiped with lattice point at all corners. A *primitive unit cell* has lattice points at corners only. A *non-primitive unit cell* has extra lattice points apart from those at the corners. In 2D, a unit cell is defined by the edge lengths *a* and *b* and the included angle γ of the parallelogram. The quantities *a*, *b* and *γ* are known as the **lattice parameters** **[7]**

i) Outline a primitive unit cell on the pattern. A primitive cell is marked with orange borders (ABCD)

ii) Measure *a*, *b*, *γ* and determine the area of the unit cell:

$a = b = 2\sqrt{2}$ cm $\gamma = 90^\circ$ area $= a \times b = 8\ cm^2$

iii)The choice of a unit cell is not unique. Outline a primitive unit cell of different shape and measure *a*, *b*, *γ*:

(FCGH) another primitive unit cell is marked with blue

$a = 2\sqrt{2}$ cm
$b = 4$ cm $\gamma = 45^\circ$

area of a parallelogram
$ab\sin\theta = 4 \times 2\sqrt{2} \times \frac{1}{\sqrt{2}} = 8\ cm^2$

iv) How is the area of your second primitive unit cell related to that of your first choice?

Area of second primitive cell is equal to area of first primitive cell

v) Now outline a non-primitive unit cell. Label *a*, *b* and *γ* and find the area.

Non-primitive unit cell is marked in green. $a = b = 4$ cm $\gamma = 90^\circ$
area $= a \times b = 4 \times 4 = 16\ cm^2$ (EACF)

vi) How does the area of nonprimitive cell relate to the area of the primitive cell?

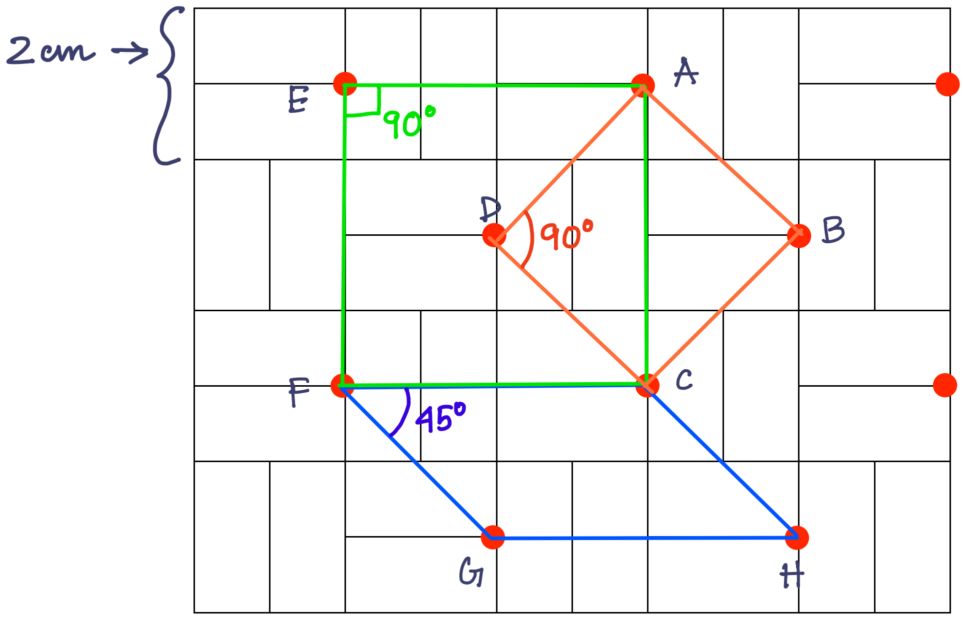
area of nonprimitive cell $= 2 \times$ area of the primitive cell.

vi) What are the number of effective lattice points in non-primitive cells?

Number of effective lattice points = 2

c) Motif: A motif is the unit of the pattern associated with a lattice point. The choice of a motif is not unique. One way is to select the contents of a primitive unit cell as a motif. The whole pattern is always generated by repetition of a suitably selected motif at all the points of the lattice.

Determine the number of tiles that are contained in the motif? **[1]**



Footpath Tiling Outside Academic Complex West

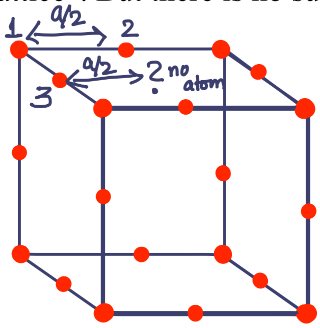
B. Three-Dimensional Crystals

B1 There are fourteen Bravais lattices. Each lattice has a conventional unit cell. Ball and spoke model these unit cells are provided. Examine these models and identify them. [15]

S. No.	Characteristic symmetry	Crystal system	Conventional Unit cell Parameters	Centering (P/I/F/S/R)	Bravais Lattice
1	None	Triclinic	$a \neq b \neq c, \alpha \neq \beta \neq \gamma$	P	aP
2	3 - 2fold axis	Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	P	oP
3	1 - 4fold axis	Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$	I	tI
4	3 - 2foldaxis	Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	C	oC
5	3 - 2foldaxis	Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	F	oF
6	1 - 6 foldaxis	Hexagonal	$a = b \neq c$ $\alpha = \beta = 90°$ $\gamma = 120°$	P	hP
	1 - 3 fold axis	Trigonal			

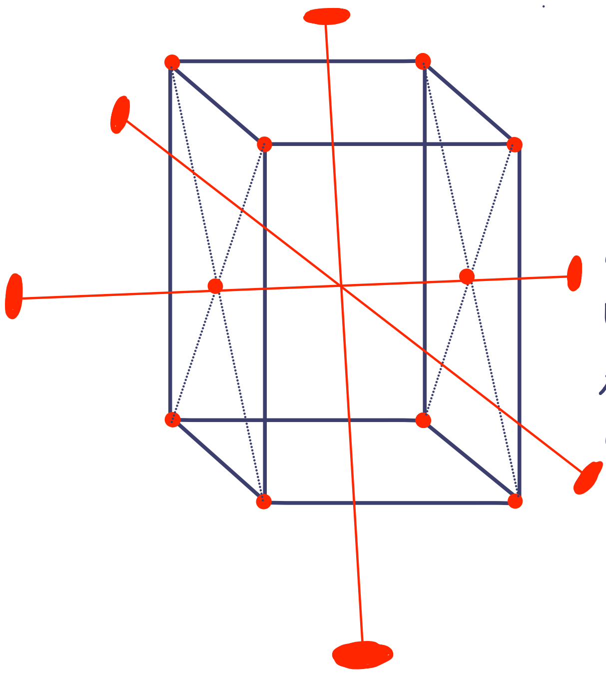
7	4 - 3fold axis	Cubic	$a=b=c$ $\alpha=\beta=\gamma=90^\circ$	I	cI
8	4 - 3fold axis	Cubic	$a=b=c$ $\alpha=\beta=\gamma=90^\circ$	P	cP
9	3 - 2fold axis	Orthorhombic	$a\neq b\neq c$ $\alpha=\beta=\gamma=90^\circ$	I	oI
10	4 - 3fold axis	Cubic	$a=b=c$ $\alpha=\beta=\gamma=90^\circ$	F	cF
11	1 - 4fold axis	Tetragonal	$a=b\neq c$ $\alpha=\beta=\gamma=90^\circ$	P	tP
12	1 - 3fold axis	Trigonal.	$a=b=c$ $\alpha=\beta=\gamma\neq 90^\circ$	R	hR
13	1 - 2fold axis	Monoclinic	$a\neq b\neq c$ $\alpha=\beta=90^\circ\neq\gamma$	C	mC
14	1 - 2fold axis	Monoclinic	$a\neq b\neq c$ $\alpha=\beta=90^\circ\neq\gamma$	P	mP

B2. In the space below, draw a primitive cubic (*cP*) unit cell. Add additional points at mid-point of the edges of the unit cell. We have thus created a unit cell of a possible "edge-centred lattice". But there is no such lattice in the list of Bravais lattices. Explain. [2]



New set of points doesnot form a lattice because the lattice points in this system does not have identical surroundings.
For example: point 1 doesnot have same surroundings as point 3

B3. Draw a unit cell of primitive tetragonal (*tP*) lattice. Add additional lattice points on the centres of a pair of rectangular faces to convert it to a unit cell of an end-centred tetragonal (*tS*) lattice. But there is no *tS* lattice in the list of 14 Bravais lattice. Explain. [3]



First with the addition of points the 4 fold symmetry of tetragonal is destroyed. We have 3 two fold axis. Also if we draw additional unit cells along it we can see that it forms end-centered orthorhomic