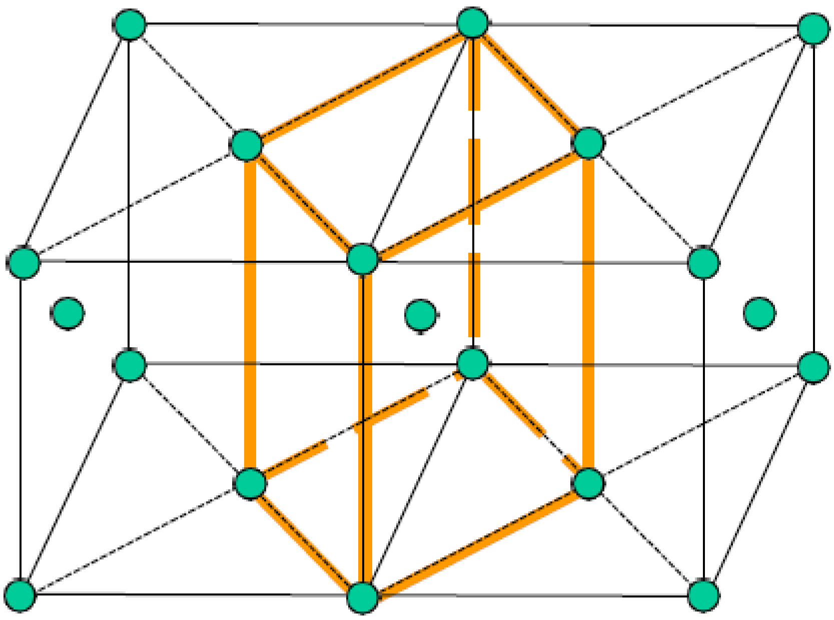
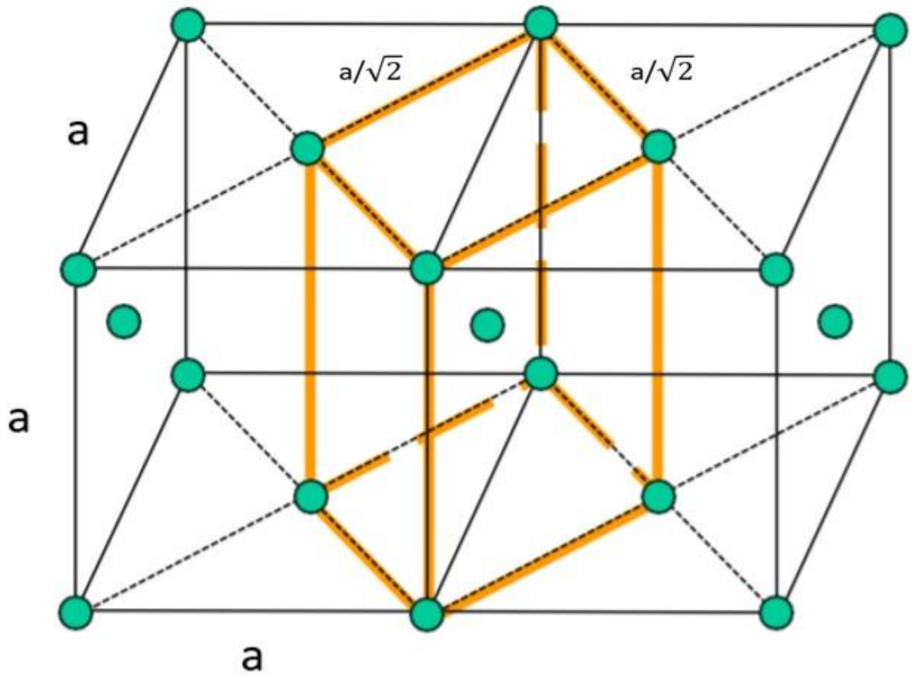
Problem 1:

(i)

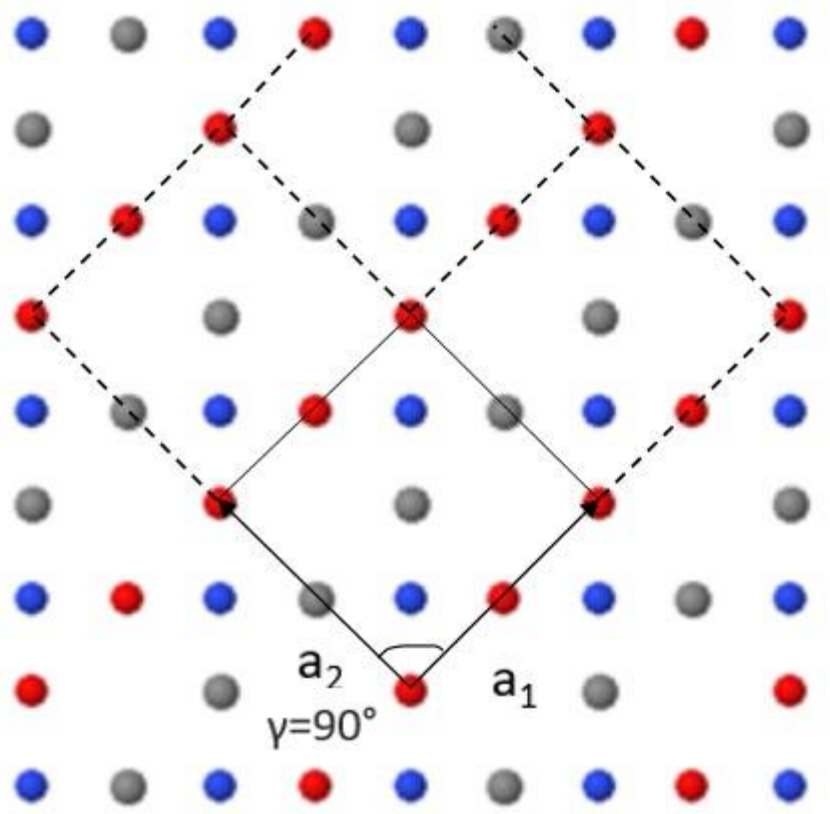


(a) Body centred tetragonal (BCT)
(b) Yes, it falls in the Bravais lattice
(c) Yes, the FCC cell possessing higher symmetry is a special case of BCT. For BCT, a=b ≠c. FCC unit cell can only be drawn from BCT when, for BCT, a=b=c/(√2) i.e., c/a for BCT should be √2 in this case.



(ii)

(a)



Red- corners: 4*(1/4)= 1

Faces: 2*(1/2)= 1

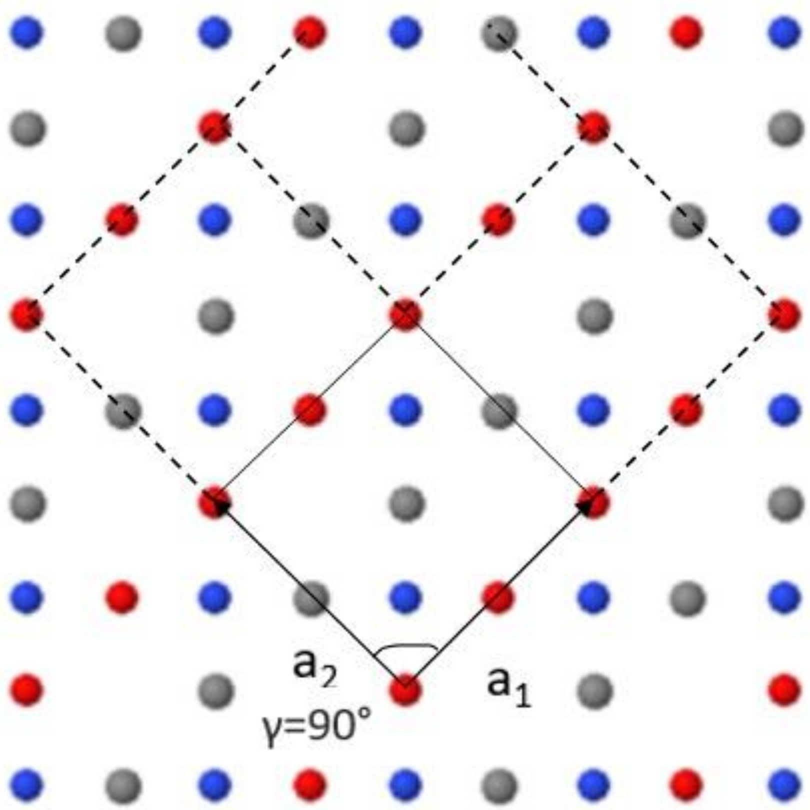
Grey- faces: 2*(1/2)= 1

Centre: 1*1= 1

Blue- inside: 2*1= 2

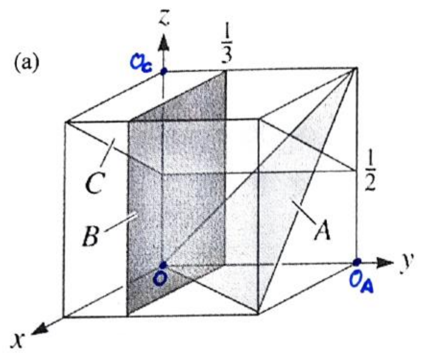
Total 6 atoms are present in primitive unit cell.

(b) a1 = a2, gamma = 90°



Problem 2:

Problem 2 : Determine the Miller indices for the planes shown in the figures below :



For plane A, we consider O_A as the origin of the coordinate system since the plane passes through the origin O.

∴ with respect to origin O_A, we have :

	x	y	z
Intercepts : (in units of basis vectors)	1	-1	1
Reciprocal of intercepts :	1	-1	1
Reduction :	<not necessary>		

Hence, Miller indices for plane A = $(1\,\bar{1}\,1)$

For plane B, we consider the point O as the origin of the coordinate system.

∴ with respect to origin O, we have :

	x	y	z
Intercepts : (in units of basis vectors)	∞	$1/3$	∞
Reciprocal of intercepts :	0	3	0
Reduction :	<not necessary>		

Hence, Miller indices for plane B = $(0\,3\,0)$

For plane C, we consider O_c as the origin of the coordinate system

$\therefore$ with respect to origin O_c, we have:

	x	y	z
Intercepts (in terms of basis vectors) :	1	∞	$-1/2$
Reciprocal of intercepts :	1	0	-2
Reduction :	<not necessary>		

Hence, Miller indices for plane C = $(1\ 0\ \bar{2})$

	x	y	z
Intercepts (in units of basis vector) :	-1	$1/2$	$3/4$
Reciprocal of intercepts :	-1	2	$\frac{4}{3}$
Reduction :	-3	6	4

Hence, Miller indices of plane A = $(\bar{3}\,6\,4)$

For plane B, considering the point O_B as the origin of the coordinate system.

$\therefore$ with respect to origin O_B, we have:

	x	y	z
Intercepts (in units of basis vector) :	1	$-3/4$	∞
Reciprocal of intercepts :	1	$-4/3$	0
Reduction :	3	-4	0

Hence, Miller indices of plane B = $(3\,\bar{4}\,0)$

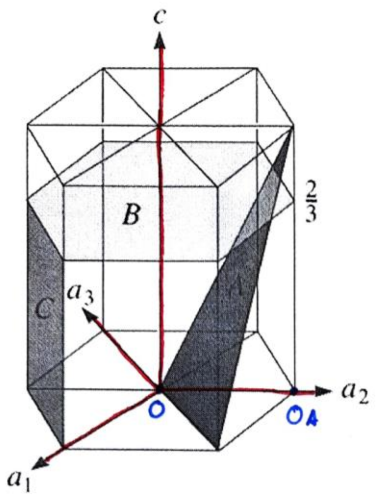
For plane C, we consider the point O as the origin of the coordinate system.

∴ with respect to origin O, we have :

	x	y	z
Intercepts (in units of basis vectors) :	2	$\frac{3}{2}$	1
Reciprocal of intercepts :	$\frac{1}{2}$	$\frac{2}{3}$	1
Reduction :	$\frac{1}{2} \times 6 = 3$	$\frac{2}{3} \times 6 = 4$	$1 \times 6 = 6$

∴ Miller indices of plane C = $(3\ 4\ 6)$

(c)



For plane A, we consider the point O_A as the origin of the coordinate system since the plane passes through the global origin O.

$\therefore$ with respect to the origin O_A, we have :

	a_1	a_2	a_3	c
Intercepts (in units of basis vectors) :	1	-1	∞	1
Reciprocal of intercepts :	1	-1	0	1
Reduction :	<not necessary>			

Hence, Miller indices of plane A = $(1\,\bar{1}\,0\,1)$ in 4 index notation
OR $(1\,\bar{1}\,1)$ in 3 index notation

For plane B, we choose point O as the origin of the coordinate system.

$\therefore$ with respect to point O, we have,

	a_1	a_2	a_3	c
Intercepts (in units of basis vectors) :	∞	∞	∞	$\frac{2}{3}$
Reciprocal of intercepts :	0	0	0	$3/2$
Reduction :	0	0	0	3

Hence, Miller indices of plane B = (0003) in 4 index notation
OR (003) in 3 index notation

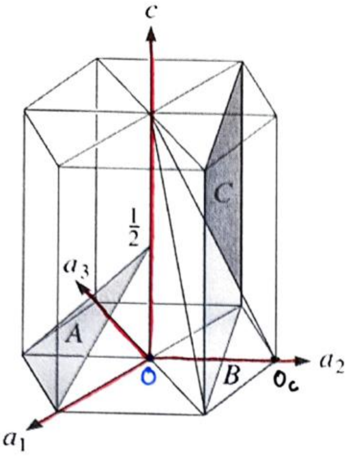
For plane C, we keep the point O as the origin of the coordinate system.

$\therefore$ with respect to point O, we have

		$\underline{a_1}$	$\underline{a_2}$	$\underline{a_3}$	$\underline{c}$
Intercepts (in units of basis vectors)	:	1	−1	∞	∞
Reciprocal of intercepts	:	1	−1	0	0
Reduction	:	<not necessary>			

Hence, Miller indices of plane C = $(1\,\bar{1}\,0\,0)$ in 4 index notation
OR $(1\,\bar{1}\,0)$ in 3 index notation

(d)



For plane A, considering point O as the origin of the coordinate system.

$\therefore$ With respect to origin O, we have:

		a_1	a_2	a_3	c
Intercepts (in units of basis vectors)	:	1	-1	∞	$\frac{1}{2}$
Reciprocal of intercepts	:	1	-1	0	2
Reduction	:	<not necessary>			

Hence, Miller indices of plane A = $(1\ \bar{1}\ 0\ 2)$ in 4 index notation
OR $(1\ \bar{1}\ 2)$ in 3 index notation

For plane B, considering the same point O as the origin of the coordinate system,

$\therefore$ with respect to origin O, we have:

		a_1	a_2	a_3	c
Intercepts (in units of basis vectors)	:	∞	1	-1	1
Reciprocal of intercepts	:	0	1	-1	1
Reduction	:	<not necessary>			

Hence, Miller indices of plane B = $(0\ 1\ \bar{1}\ 1)$ in 4 index notation
OR $(0\ 1\ 1)$ in 3 index notation

For plane C, choosing point O as the origin of the coordinate system.

$\therefore$ with respect to origin O, we have,

		a_1	a_2	a_3	c
Intercepts (in units of basis vectors)	:	-1	$\frac{1}{2}$	-1	∞
Reciprocal of intercepts	:	-1	2	-1	0
Reduction	:	⟨not necessary⟩			

Hence, Miller indices of plane C = $(\bar{1}\ 2\ \bar{1}\ 0)$ in 4 index notation
OR $(\bar{1}\ 2\ 0)$ in 3 index notation

Alternatively,
choosing point O_c as the origin of the coordinate system, we have :

		a_1	a_2	a_3	c
Intercepts (in units of basis vectors)	:	1	$-\frac{1}{2}$	1	∞
Reciprocal of intercepts	:	1	-2	1	0
Reduction	:	⟨not necessary⟩.			

Hence, Miller indices of plane C = $(1\ \bar{2}\ 1\ 0)$ in 4 index notation
OR $(1\ \bar{2}\ 0)$ in 3 index notation

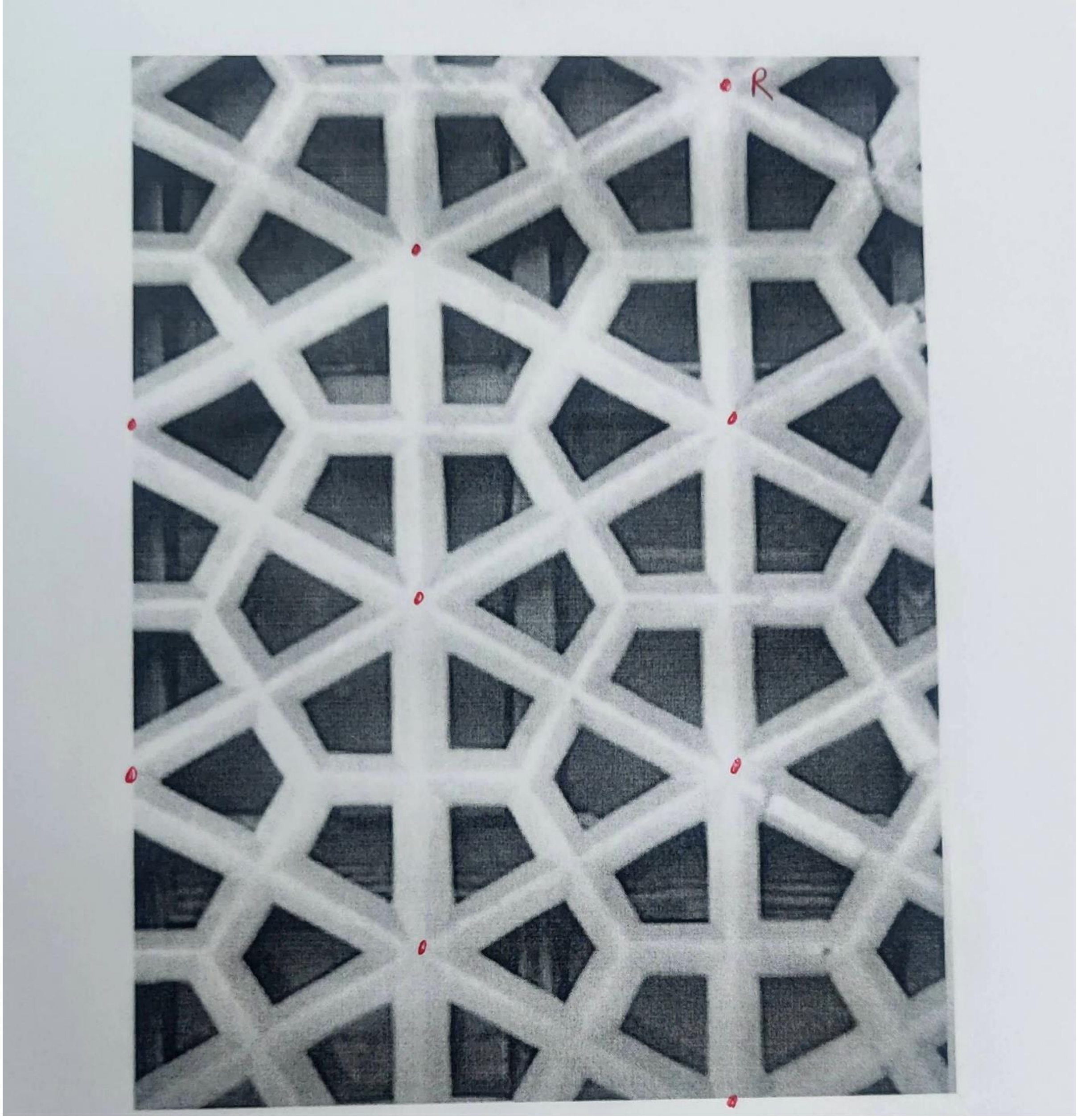
Problem 3:

(a) A M T U – vertical mirror plane only.
B C D - horizontal mirror plane only.
F G J - no symmetry
H I O - both vertical and horizontal mirror plane and 2-fold axis of rotation
N S - 2-fold axis of rotation

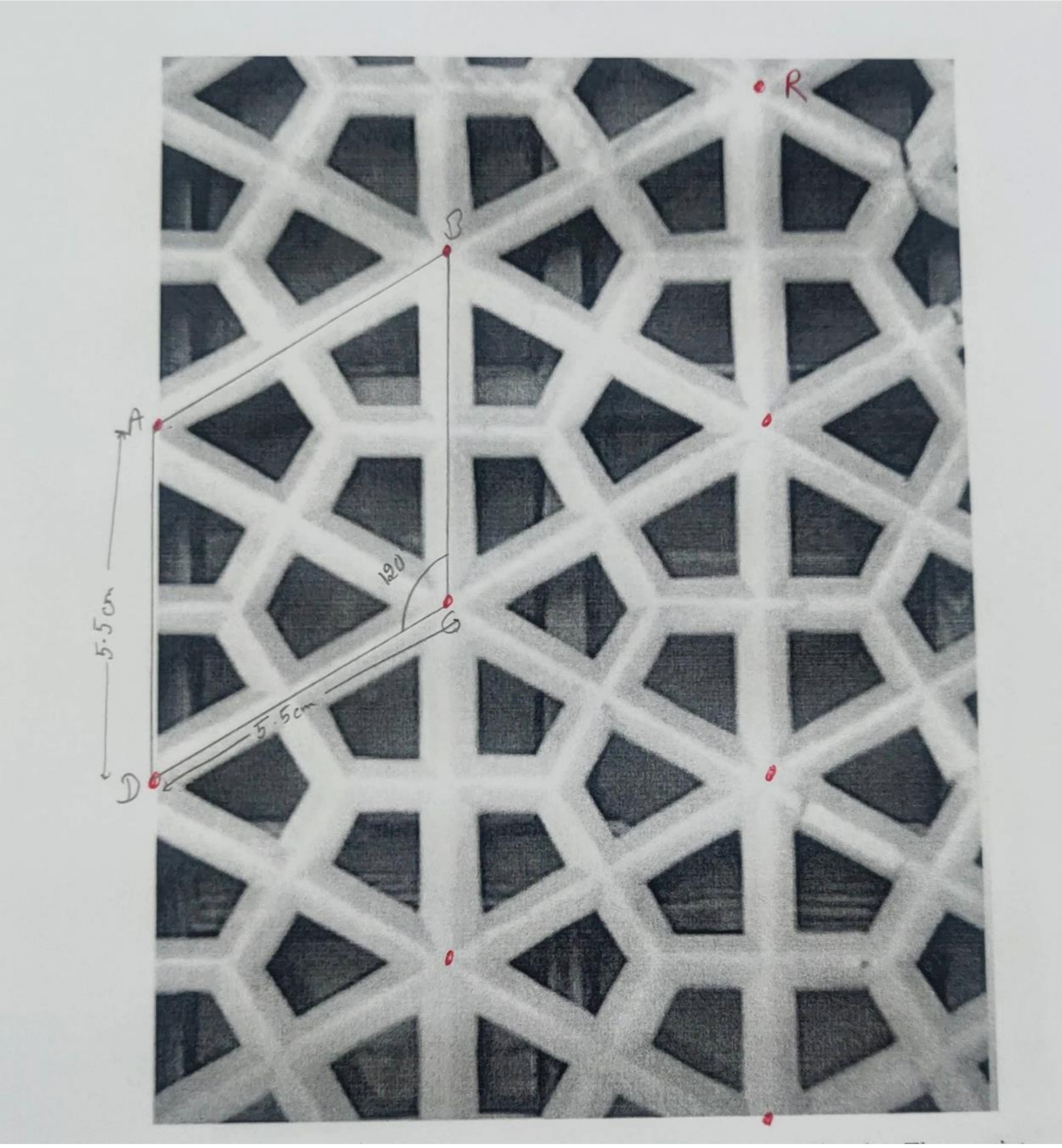
(b) A M T U **V W Y**
B C D **E K**
F G J **L P Q R**
H I O **X**
N S **Z**

Problem 4:

(a, b)



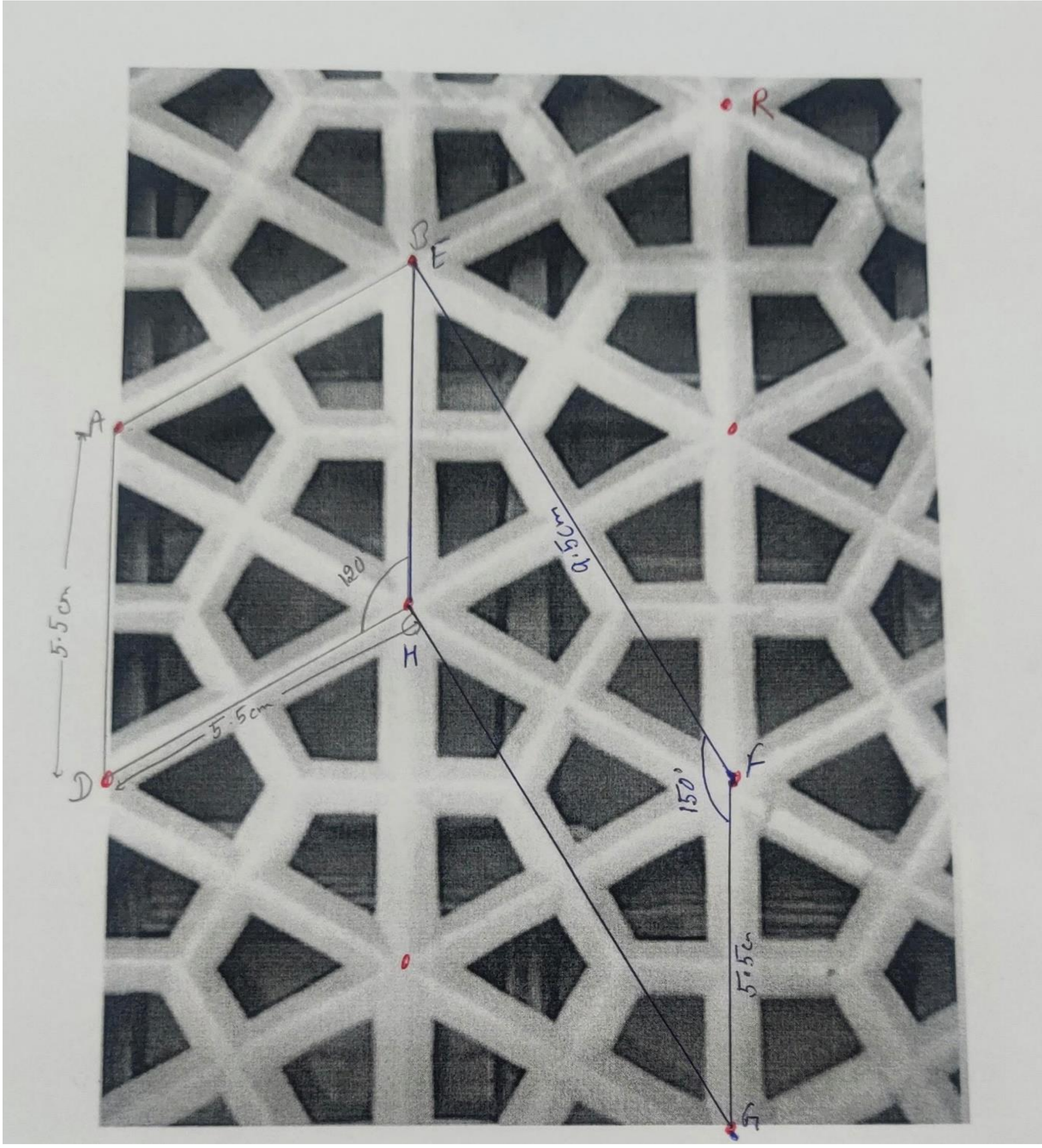
(c)



a = b = 5.5 cm and α = 120°.

Area = anywhere between 24 to 27 cm^2.

(d)

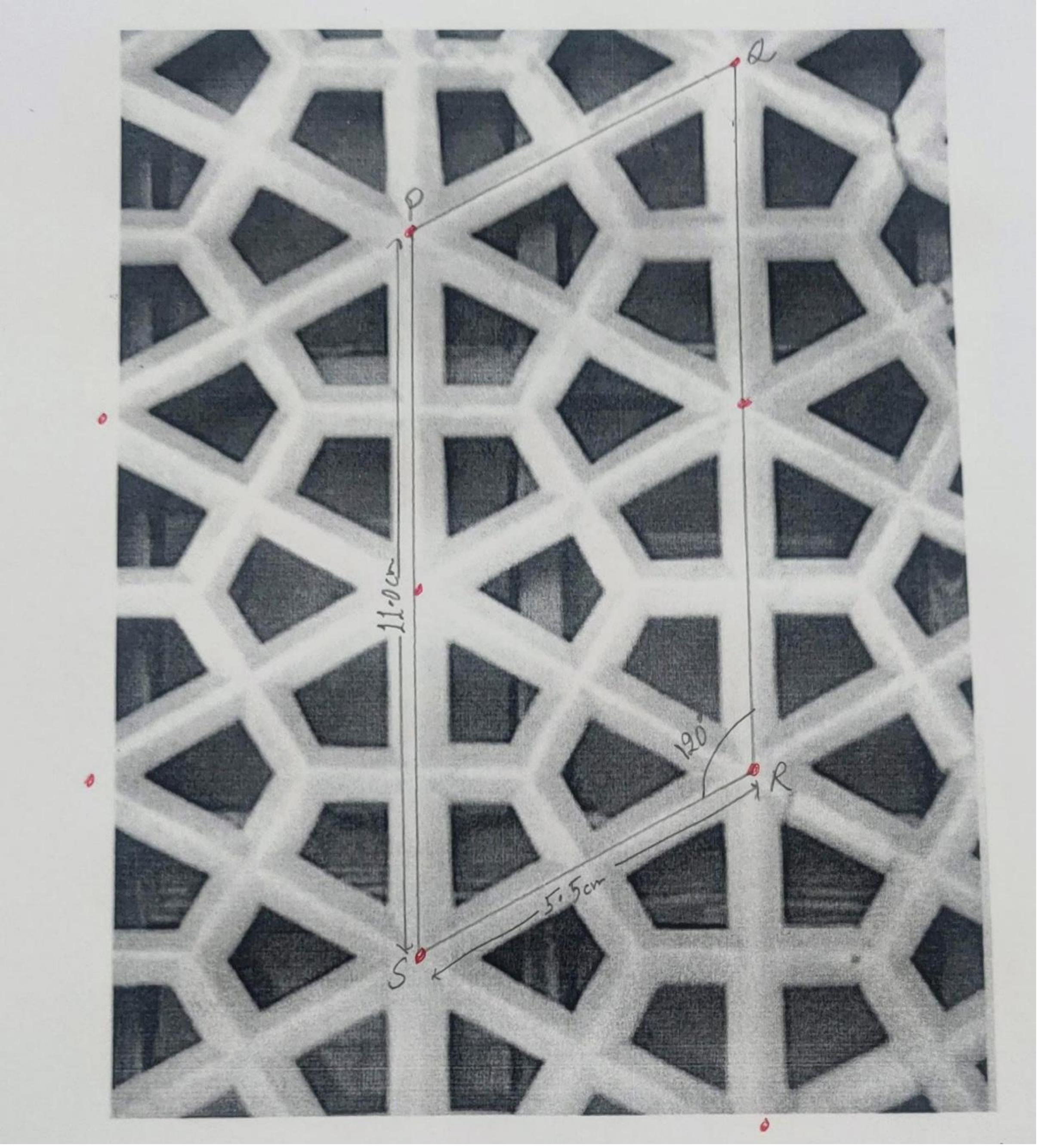


a = 9.5 cm, b = 5.5 cm and γ = 150°.

Area = anywhere between 24 to 27 cm^2.

(e) The area of both the primitive unit cells are almost equal. Since, both have same number of effective numbers of lattice points i.e., 1.

(f)



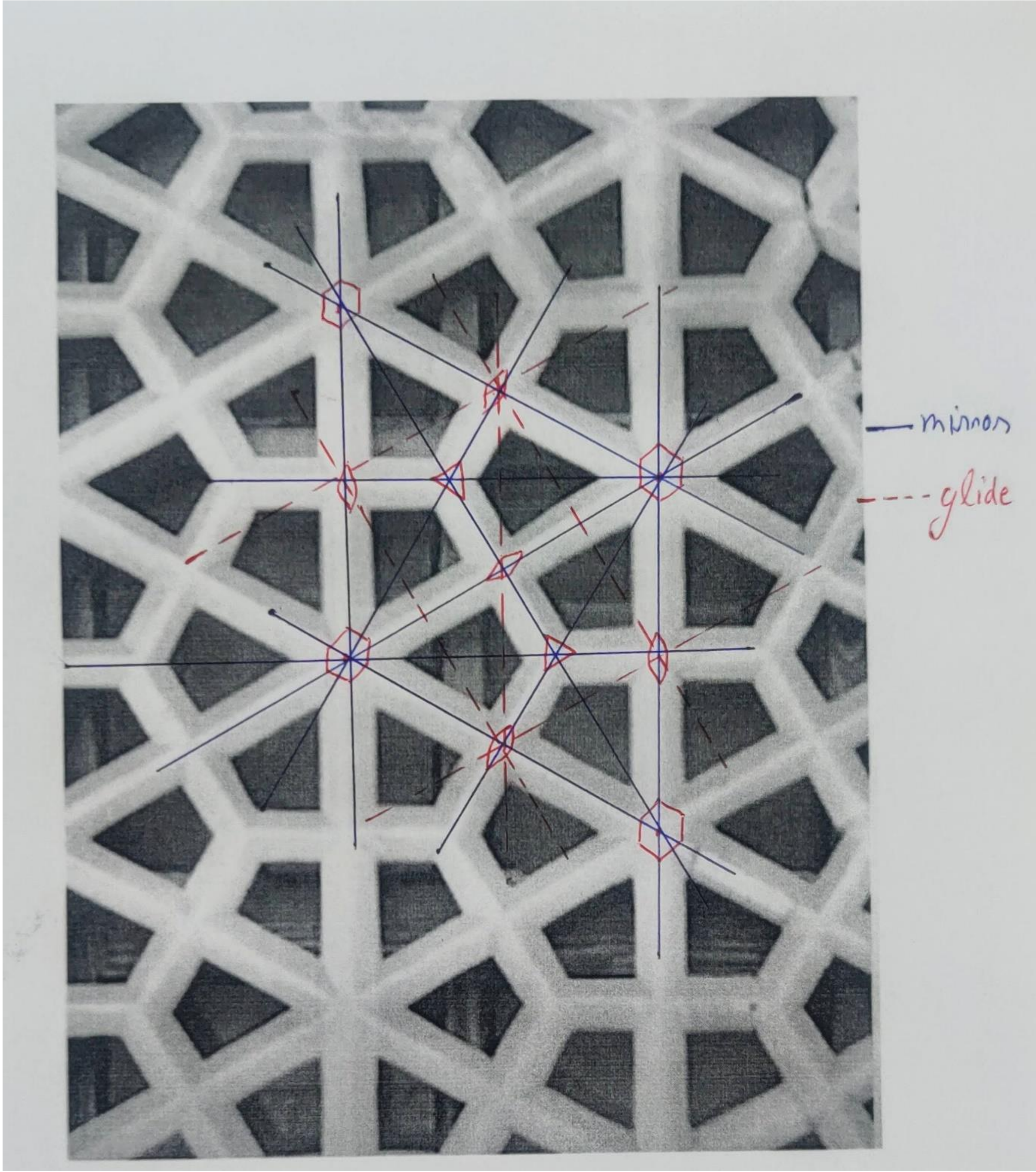
a = 11.0 cm, b = 5.5 cm and γ = 120°.

Area = anywhere between 49 to 53 cm^2.

The area of non-primitive unit cell is almost double of the area of primitive unit cell.

The area of a unit cell is directly proportional to the effective number of lattice points. Since, non-primitive unit cell has 2 effective number of lattice points, as compared to the primitive unit cell having 1 effective number of lattice points

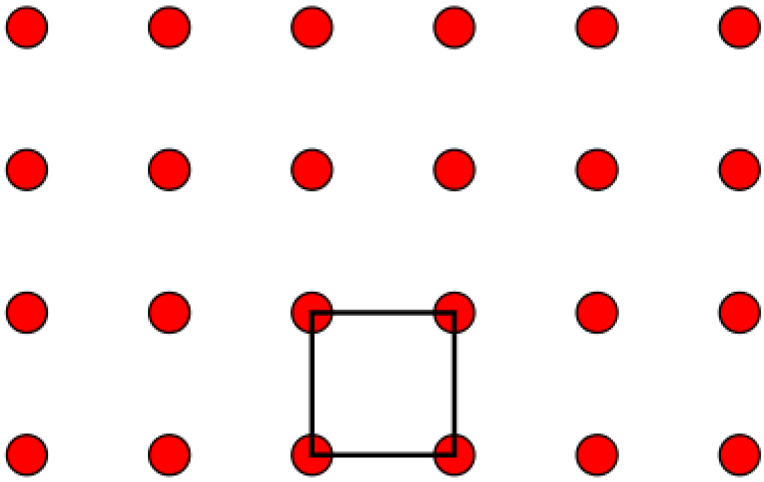
(g, h)



p6mm

Problem 5:

(a)



Out of all the parallelograms, square is considered as the unit cell because the volume is the smallest and it provides the most symmetry.

(b) Unit cell is a small volume of the crystal which by periodic repetition generates the entire crystal without overlaps or gaps. The repetition of such triangular unit cells generates the entire crystal with gaps. Therefore, triangular unit cells cannot be selected as the unit cell.

(c) The unit cell shown is primitive because of the existence of more than one atom exists in the motif.

(d) No. of lattice points in the unit cell= 4

$$8 * \left(\frac{1}{8}\right) + 4 * \left(\frac{1}{2}\right) + 1 * 1$$