

Motivation for our Patterson Lab

- We want to calculate an electron density map for proteinase K and see the shape of the molecule. We get this map by taking the Fourier transform of the structure factors:

$$\rho(xyz) = \sum |F_{hkl}| \cos 2\pi(hx + ky + lz - \alpha_{hkl})$$

- We have measured intensities of the native ProK crystal. $\sqrt{I_{hkl}} = |F_{hkl}|$
- The phases, α_{hkl} , will come from an isomorphous replacement experiment.
- We soaked ProK crystals in heavy atom compounds PCMBS, EuCl_3 , or GdCl_3 in hope the metals would bind to proteinase K.
 - 3 native data sets
 - 8 PCMBS data sets
 - 4 EuCl_3 data sets
 - 3 GdCl_3 data sets
- A difference Patterson map will provide clues to help us determine the coordinates (x,y,z) of the heavy atoms. The primary goal of this lab is to follow the trail of clues to reveal the heavy atom coordinates.

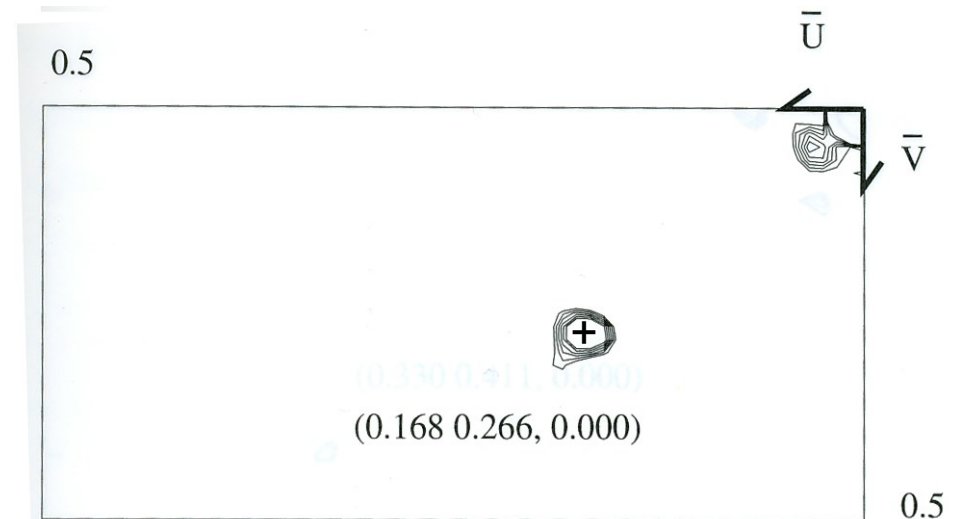


Note for Mikey in 2023

- Students asked lots of questions. Great!
- Slowed down to permit questions.
- As a result, I didn't cover all material. Ran out of time. Got to slide 34. 6 slides to go.
- I think this was much better than Patterson lab 2021. It's OK that I didn't finish delivering the presentation. I feel the students could follow at the slower speed. Jeffrey says he doesn't have full grasp, but will review.
- Next year, clean up end of presentation on ProK. Too much text.

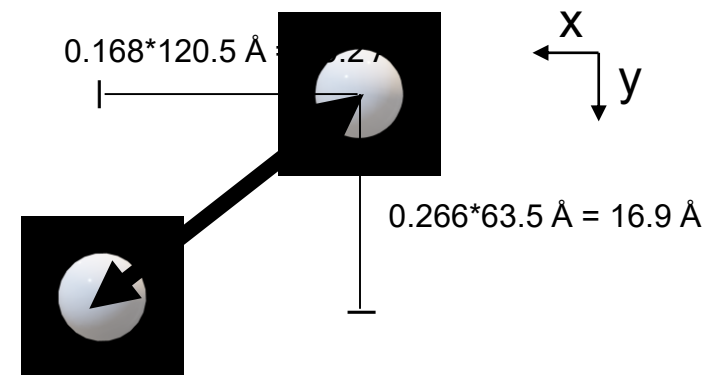
Each difference Patterson map reveals the relative positions of a pair of atoms in the unit cell

- The relative position between atoms is described as a vector.
- The vectors between atoms are encoded in the coordinates of the difference Patterson peak (u, v, w).
- For example, the peak at $u=0.158$, $v=0.266$, $w=0.00$ means that there are two atoms in the unit cell separated by a vector that is:
 - $0.168 \times a$ in the x-direction.
 - $0.266 \times b$ in the y-direction.
 - $0.000 \times c$ in the z-direction.
- This is helpful information, but it doesn't tell us the positions of the atoms relative to the unit cell origin.



Unit cell dimensions:

$a=120.5 \text{ \AA}$, $b=63.5 \text{ \AA}$, $c=38.2 \text{ \AA}$, $\alpha=\beta=\gamma=90^\circ$



Symmetry operators describe the positions of atoms relative to the origin.

- Knowledge of the symmetry equivalent positions can help us determine the coordinates of the heavy atom relative to the origin.
- For example, in $P2_12_12$, there are four symmetry operators.

$$(1) \quad x, \quad y, \quad z$$

$$(2) \quad -x, \quad -y, \quad z$$

$$(3) \quad -x + \frac{1}{2}, \quad y + \frac{1}{2}, \quad -z$$

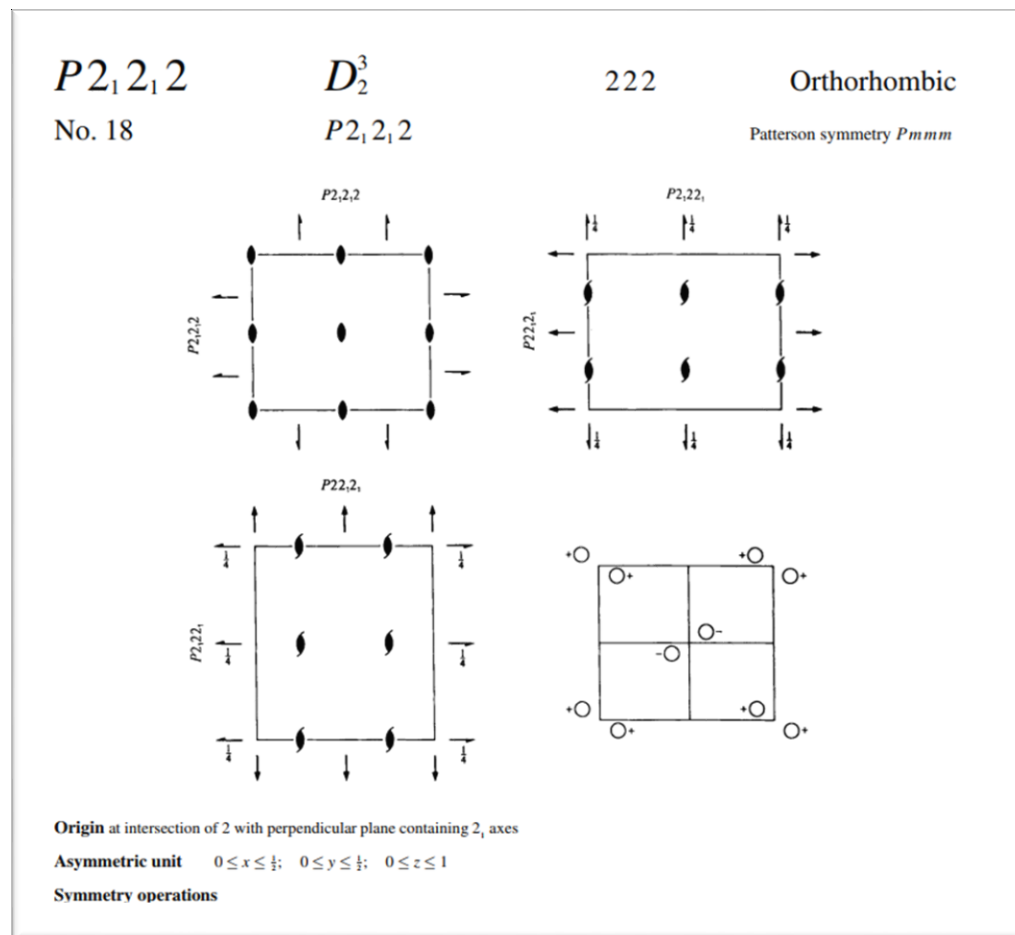
$$(4) \quad x + \frac{1}{2}, \quad -y + \frac{1}{2}, \quad -z$$

- Hence, an atom located at x, y, z coordinate 0.1, 0.2, 0.3, must have symmetry copies located at the following 3 sites

$$\bullet \quad -0.1, -0.2, \quad 0.3$$

$$\bullet \quad 0.4, \quad 0.7, \quad -0.3$$

$$\bullet \quad 0.5, \quad 0.3, \quad -0.3$$



Differences between symmetry equivalent positions equate Patterson vectors to the atomic coordinates.

For example, we have seen space group $P2_12_12$ has 4 symmetry equivalent positions:

$$(1) \quad x, \quad y, \quad z$$

$$(2) \quad -x, \quad -y, \quad z$$

$$(3) \quad -x+\frac{1}{2}, \quad y+\frac{1}{2}, \quad -z$$

$$(4) \quad x+\frac{1}{2}, \quad -y+\frac{1}{2}, \quad -z$$

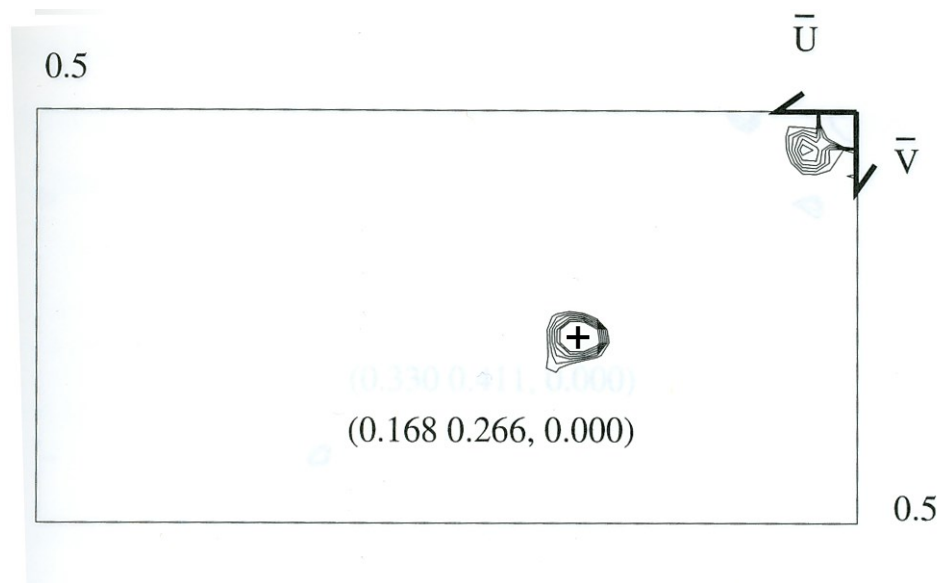
To define the vector between an atom at position 1 and position 2 we simply take the difference between their symmetry equivalent positions 1 and 2:

$$1. \quad X, \quad Y, \quad Z$$

$$2. \quad -X, \quad -Y, \quad Z$$

$$u=2x, \quad v=2y, \quad w=0$$

Now we have an equation relating the Patterson peak coordinate u,v,w to the heavy atom position in the unit cell, x,y,z .



Plug in u to solve for x

$$0.168=2x$$

$$0.084=x$$

Plug in v to solve for y

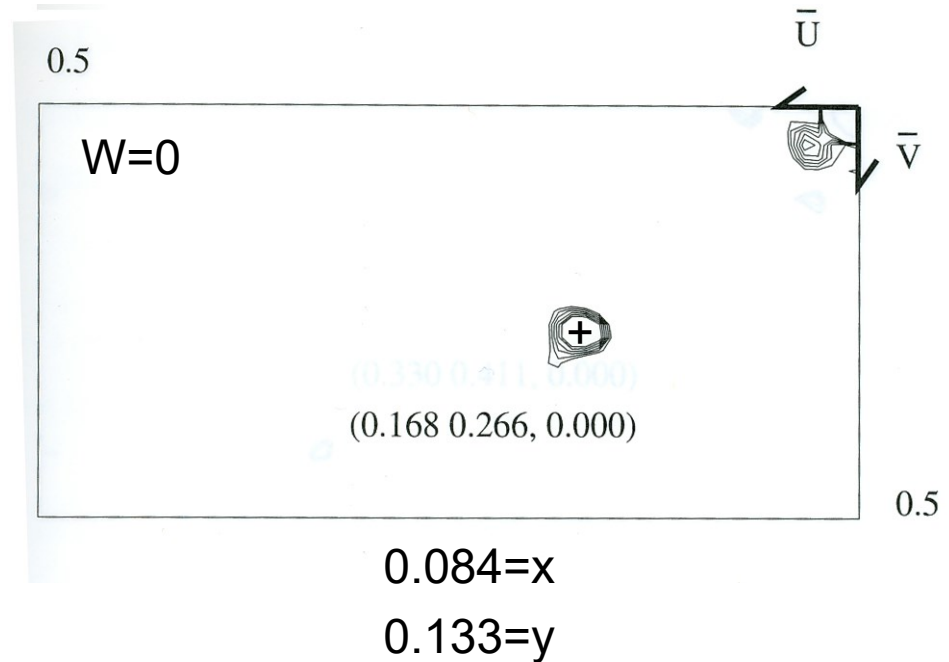
$$0.266=2y$$

$$0.133=y$$

The only remaining task is to determine the coordinate, z .

What is the value of z?

$$\begin{array}{l} 1. \quad X, \quad Y, \quad Z \\ 2. \quad \underline{-X, \quad -Y, \quad Z} \\ u=2x, \quad v=2y, \quad w=0 \end{array}$$



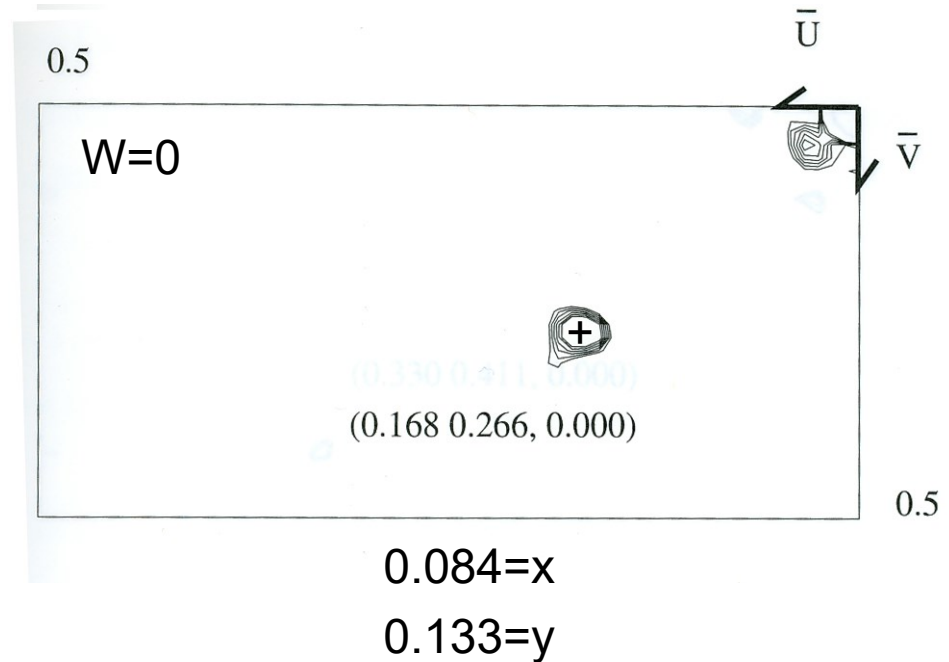
a) Zero

b) x/y

c) not specified by this map section.

What is the value of z?

$$\begin{array}{l} 1. \quad X, \quad Y, \quad Z \\ 2. \quad \underline{-X, \quad -Y, \quad Z} \\ u=2x, \quad v=2y, \quad w=0 \end{array}$$



a) Zero

b) x/y

c) not specified by this map section.

How can we determine the z coordinate?

Many more Patterson peaks are expected in space group $P2_12_12$. How many?

		1	2	3	4
	Symmetry ops	x y z	-x -y z	-x+½ y+½ -z	x+½ -y+½ -z
1	x y z	1-1	2-1	3-1	4-1
2	-x -y z	1-2	2-2	3-2	4-2
3	-x+½ y+½ -z	1-3	2-3	3-3	4-3
4	x+½ -y+½ -z	1-4	2-4	3-4	4-4

How many of these peaks are off-origin?

		1	2	3	4
	Symmetry ops	x y z	-x -y z	-x+½ y+½ -z	x+½ -y+½ -z
1	x y z	$\begin{array}{rrr} x & y & z \\ \hline -x & -y & -z \\ \hline 0 & 0 & 0 \end{array}$	$\begin{array}{rrr} -x & -y & z \\ \hline -x & -y & -z \\ \hline -2x & -2y & 0 \end{array}$	$\begin{array}{rrr} -x+\frac{1}{2} & y+\frac{1}{2} & -z \\ \hline -x & -y & -z \\ \hline -2x+\frac{1}{2} & \frac{1}{2} & -2z \end{array}$	$\begin{array}{rrr} x+\frac{1}{2} & -y+\frac{1}{2} & -z \\ \hline -x & -y & -z \\ \hline \frac{1}{2} & -2y+\frac{1}{2} & -2z \end{array}$
2	-x -y z	$\begin{array}{rrr} x & y & z \\ \hline +x & +y & -z \\ \hline 2x & 2y & 0 \end{array}$	$\begin{array}{rrr} -x & -y & z \\ \hline +x & +y & -z \\ \hline 0 & 0 & 0 \end{array}$	$\begin{array}{rrr} -x+\frac{1}{2} & y+\frac{1}{2} & -z \\ \hline +x & +y & -z \\ \hline \frac{1}{2} & 2y+\frac{1}{2} & -2z \end{array}$	$\begin{array}{rrr} x+\frac{1}{2} & -y+\frac{1}{2} & -z \\ \hline +x & +y & -z \\ \hline 2x+\frac{1}{2} & \frac{1}{2} & -2z \end{array}$
3	-x+½ y+½ -z	$\begin{array}{rrr} x & y & z \\ \hline X-\frac{1}{2} & -y-\frac{1}{2} & z \\ \hline 2x-\frac{1}{2} & -\frac{1}{2} & 2z \end{array}$	$\begin{array}{rrr} -x & -y & z \\ \hline X-\frac{1}{2} & -y-\frac{1}{2} & z \\ \hline -\frac{1}{2} & -2y-\frac{1}{2} & 2z \end{array}$	$\begin{array}{rrr} -x+\frac{1}{2} & y+\frac{1}{2} & -z \\ \hline X-\frac{1}{2} & -y-\frac{1}{2} & z \\ \hline 0 & 0 & 0 \end{array}$	$\begin{array}{rrr} x+\frac{1}{2} & -y+\frac{1}{2} & -z \\ \hline X-\frac{1}{2} & -y-\frac{1}{2} & z \\ \hline 2x & -2y & 0 \end{array}$
4	x+½ -y+½ -z	$\begin{array}{rrr} x & y & z \\ \hline -X-\frac{1}{2} & y-\frac{1}{2} & z \\ \hline -\frac{1}{2} & 2y-\frac{1}{2} & 2z \end{array}$	$\begin{array}{rrr} -x & -y & z \\ \hline -X-\frac{1}{2} & y-\frac{1}{2} & z \\ \hline -2x-\frac{1}{2} & -\frac{1}{2} & 2z \end{array}$	$\begin{array}{rrr} -x+\frac{1}{2} & y+\frac{1}{2} & -z \\ \hline -X-\frac{1}{2} & y-\frac{1}{2} & z \\ \hline -2x & 2y & 0 \end{array}$	$\begin{array}{rrr} x+\frac{1}{2} & -y+\frac{1}{2} & -z \\ \hline -X-\frac{1}{2} & y-\frac{1}{2} & z \\ \hline 0 & 0 & 0 \end{array}$

In what planes do we expect difference Patterson peaks in $P2_12_12$?

		1	2	3	4
	Symmetry ops	x y z	-x -y z	-x+½ y+½ -z	x+½ -y+½ -z
1	x y z	0 0 0	-2x -2y 0	-2x+½ ½ -2z	½ -2y+½ -2z
2	-x -y z	2x 2y 0	0 0 0	½ 2y+½ -2z	2x+½ ½ -2z
3	-x+½ y+½ -z	2x-½ -½ 2z	-1/2 -2y-½ 2z	0 0 0	2x -2y 0
4	x+½ -y+½ -z	-½ 2y-½ 2z	-2x-½ -½ 2z	-2x 2y 0	0 0 0

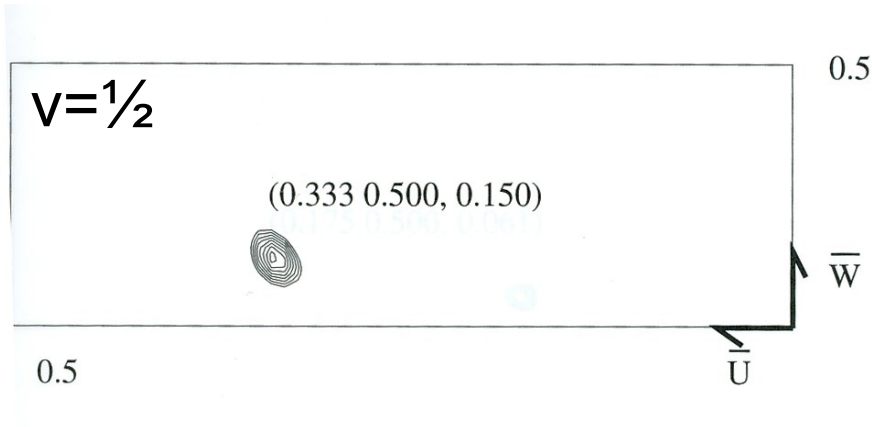
In what planes do we expect difference Patterson peaks in $P2_12_12$?

		1	2	3	4
	Symmetry ops	x y z	-x -y z	-x+½ y+½ -z	x+½ -y+½ -z
1	x y z	0 0 0	-2x -2y 0	-2x+½ ½ -2z	½ -2y+½ -2z
2	-x -y z	2x 2y 0	0 0 0	½ 2y+½ -2z	2x+½ ½ -2z
3	-x+½ y+½ -z	2x-½ -½ 2z	-1/2 -2y-½ 2z	0 0 0	2x -2y 0
4	x+½ -y+½ -z	-½ 2y-½ 2z	-2x-½ -½ 2z	-2x 2y 0	0 0 0

The utility of Harker sections

- A Harker section is a plane where we expect to find Patterson peaks arising from crystallographic symmetry such as rotation or screw axes.
- Harker sections are indicated whenever a difference between symmetry operators defines a plane (i.e. produces a constant for one of the coordinate dimensions).
- Harker sections are helpful because they can eliminate the ambiguity of assigning a Patterson peak to its corresponding symmetry equivalent positions.
 - We have 6 Patterson peaks and 6 pairs of symmetry operators – chances for an incorrect assignment are high if we made the assignments randomly.
- Incorrect assignment would lead to incorrect x,y,z coordinates.

Which of these difference vectors is likely to correspond to the difference Patterson peak shown here?



a)

$$\begin{array}{l} 1. \quad X, \quad Y, \quad Z \\ 2. \quad -X, \quad -Y, \quad Z \\ \hline u=2x, \quad v=2y, \quad w=0 \end{array}$$

b)

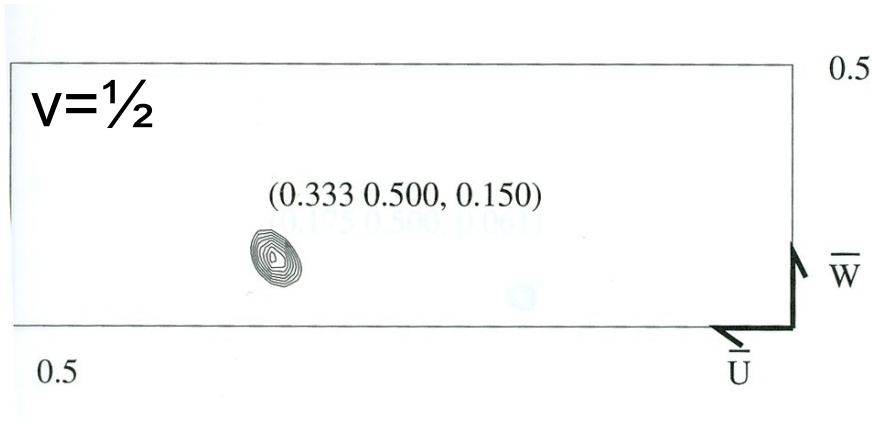
$$\begin{array}{l} 1. \quad X, \quad Y, \quad Z \\ 3. \quad \frac{1}{2}-X, \frac{1}{2}+Y, -Z \\ \hline u=2x-\frac{1}{2}, \quad v=-\frac{1}{2}, \quad w=2z \end{array}$$

c)

$$\begin{array}{l} 1. \quad X, \quad Y, \quad Z \\ 4. \quad \frac{1}{2}+X, \frac{1}{2}-Y, -Z \\ \hline u=-\frac{1}{2}, \quad v=2y-\frac{1}{2}, \quad w=2z \end{array}$$

d) They are all equally likely.

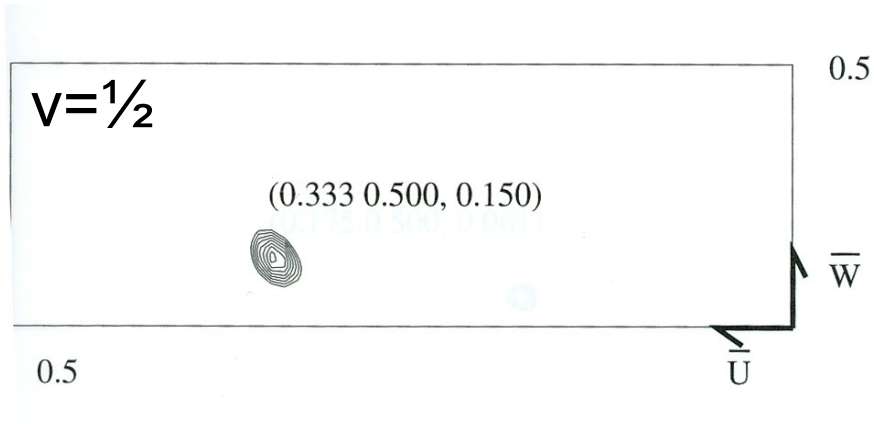
Which of these difference vectors is likely to correspond to the difference Patterson peak shown here?



b)

1.	$X,$	$Y,$	Z
3.	$\frac{1}{2}-X,$	$\frac{1}{2}+Y,$	$-Z$
	$u=2x-\frac{1}{2},$	$v=-\frac{1}{2},$	$w=2z$

Harker Section $v=1/2$



$$\begin{array}{l}
 1. \quad X, \quad Y, \quad Z \\
 3. \quad \frac{1}{2}-X, \frac{1}{2}+Y, -Z \\
 \hline
 u=2x-\frac{1}{2}, v=-\frac{1}{2}, w=2z
 \end{array}$$

Plug in u to solve for x

$$0.333=2x-1/2$$

$$0.833=2x$$

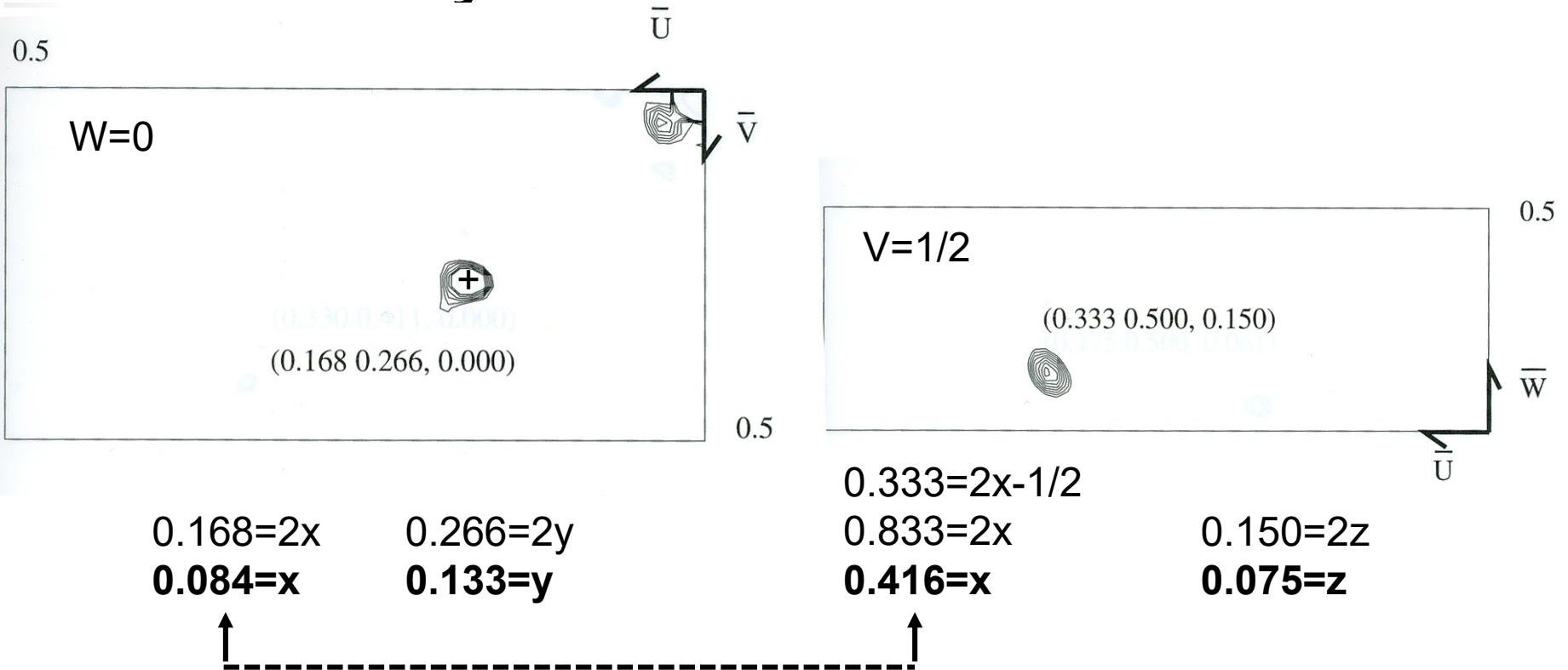
$$0.416=x$$

Plug in w to solve for z

$$0.150=2z$$

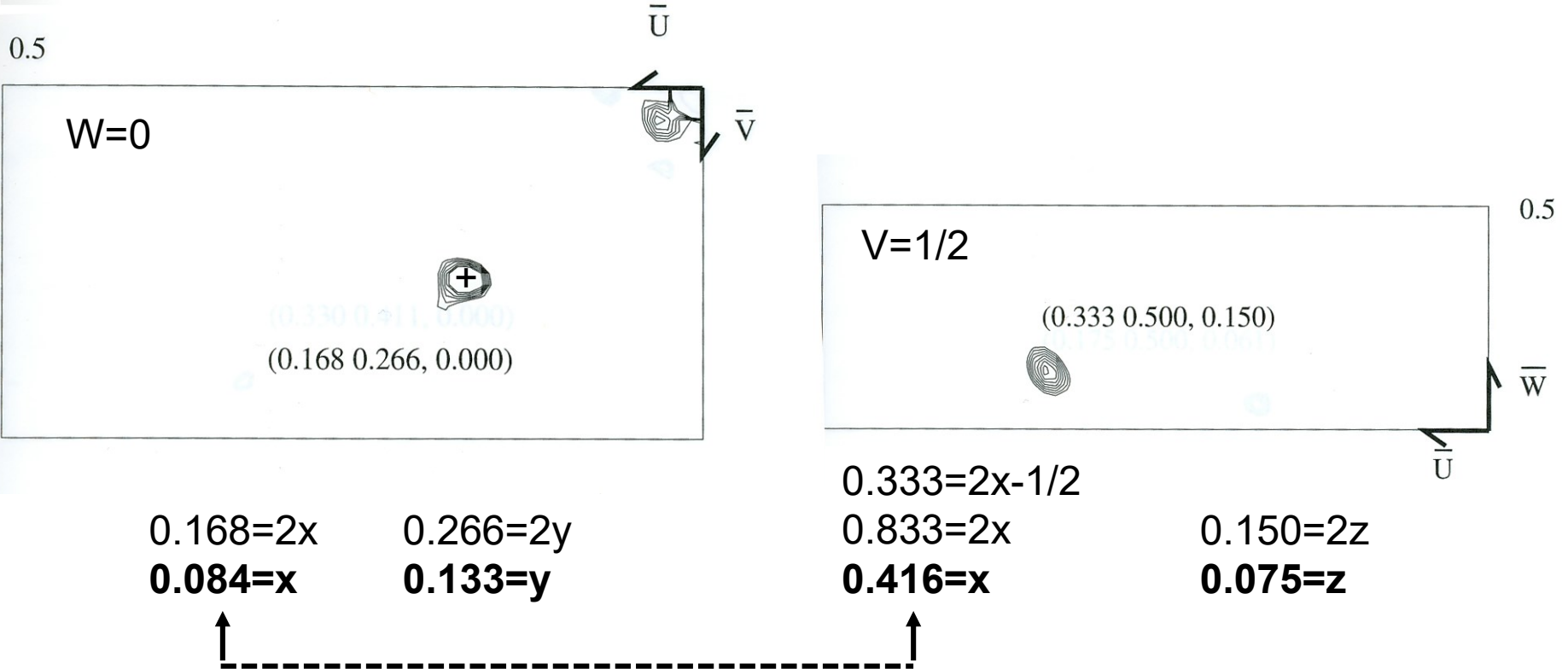
$$0.075=z$$

What are the coordinates (x,y,z) for this heavy atom?



- a) $x=0.084, y=0.133, z=0.075$
- b) $x=0.416, y=0.133, z=0.075$
- c) Either a or b is OK.

What are the coordinates x, y, z for this heavy atom?

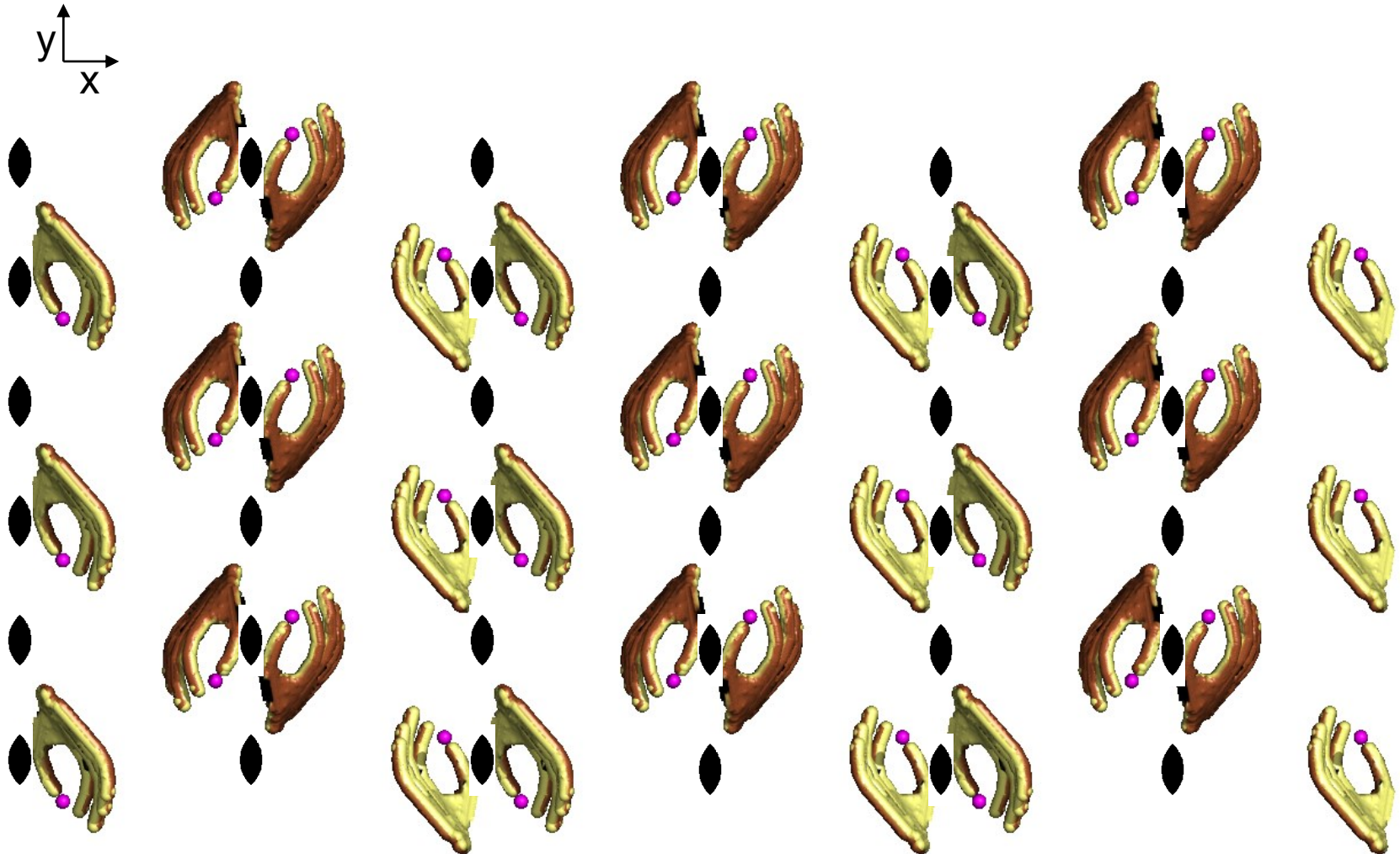


a) $x=0.084, y=0.133, z=0.075$

b) $x=0.416, y=0.133, z=0.075$

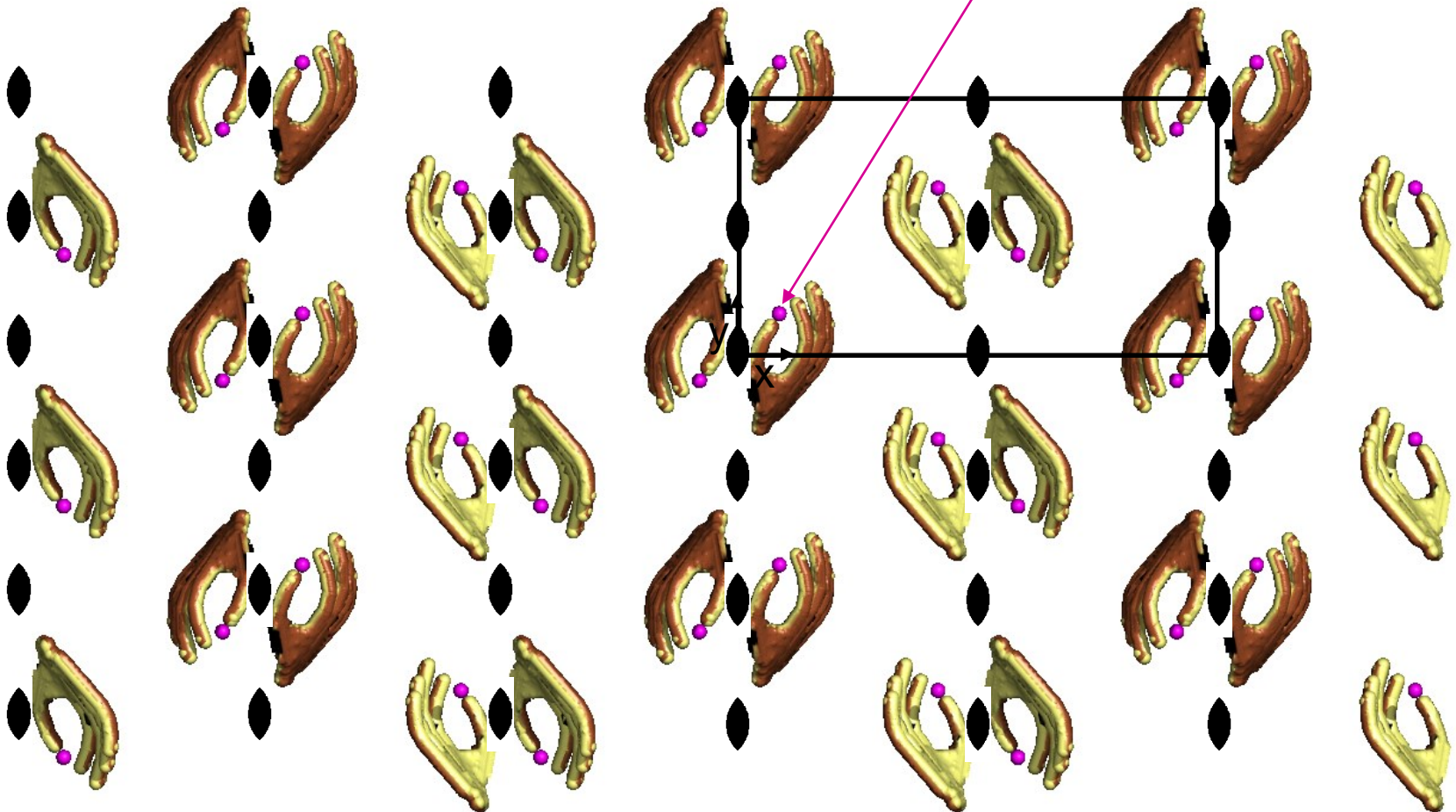
c) Either a or b is OK.

Draw the unit cell for this crystal



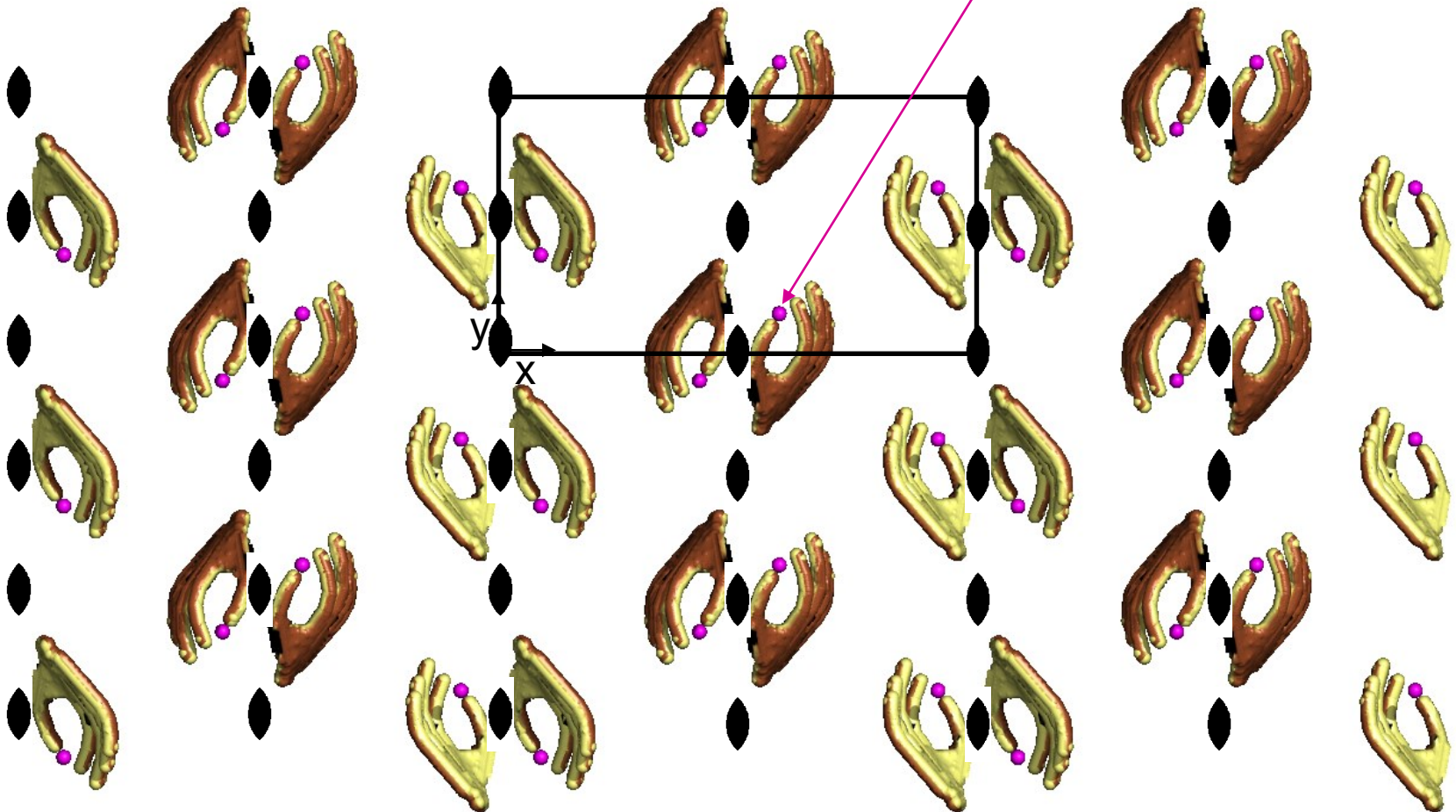
This is one valid choice of unit cell

$x=0.084, y=0.133, z=0.075$



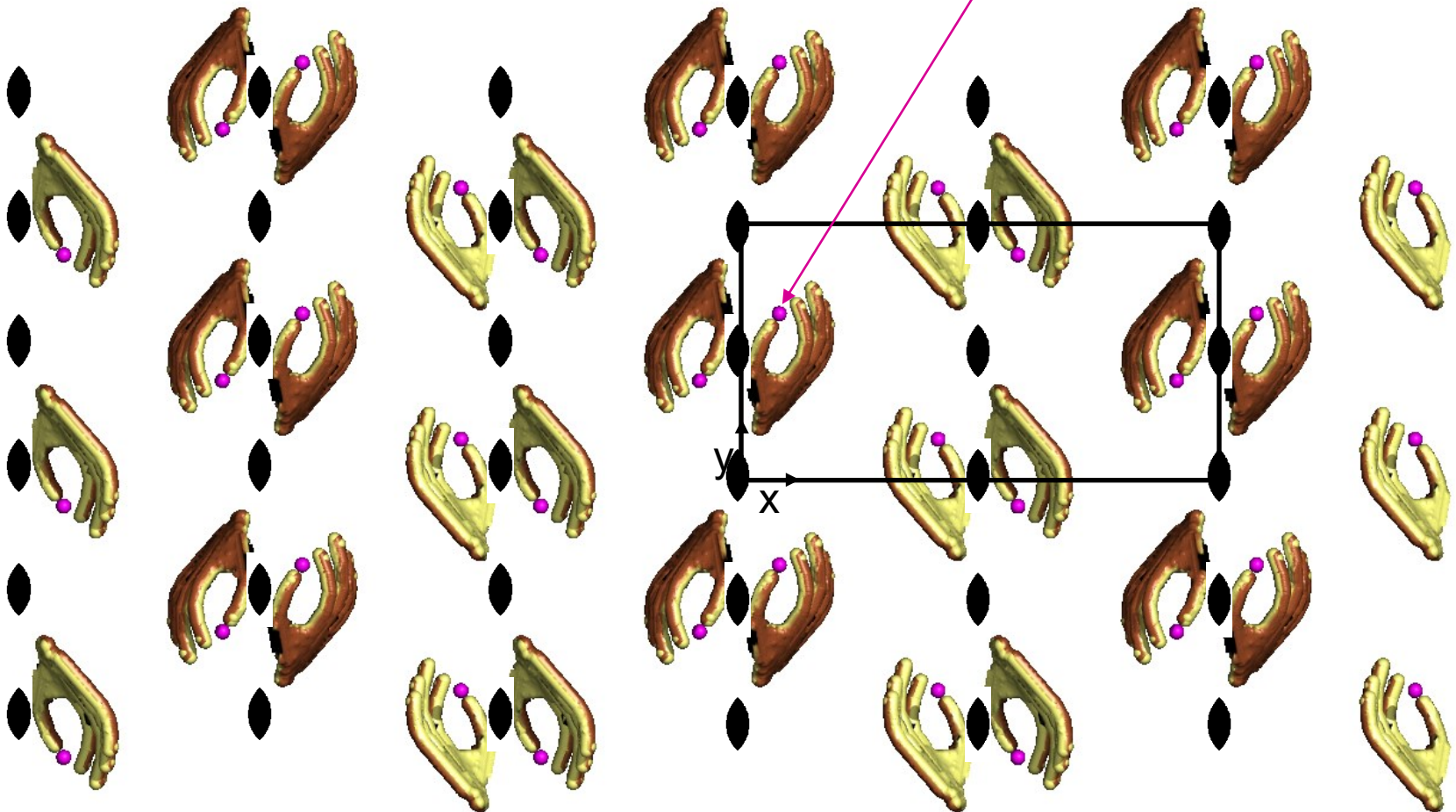
This choice of cell gives

$x=0.584, y=0.133, z=0.075$



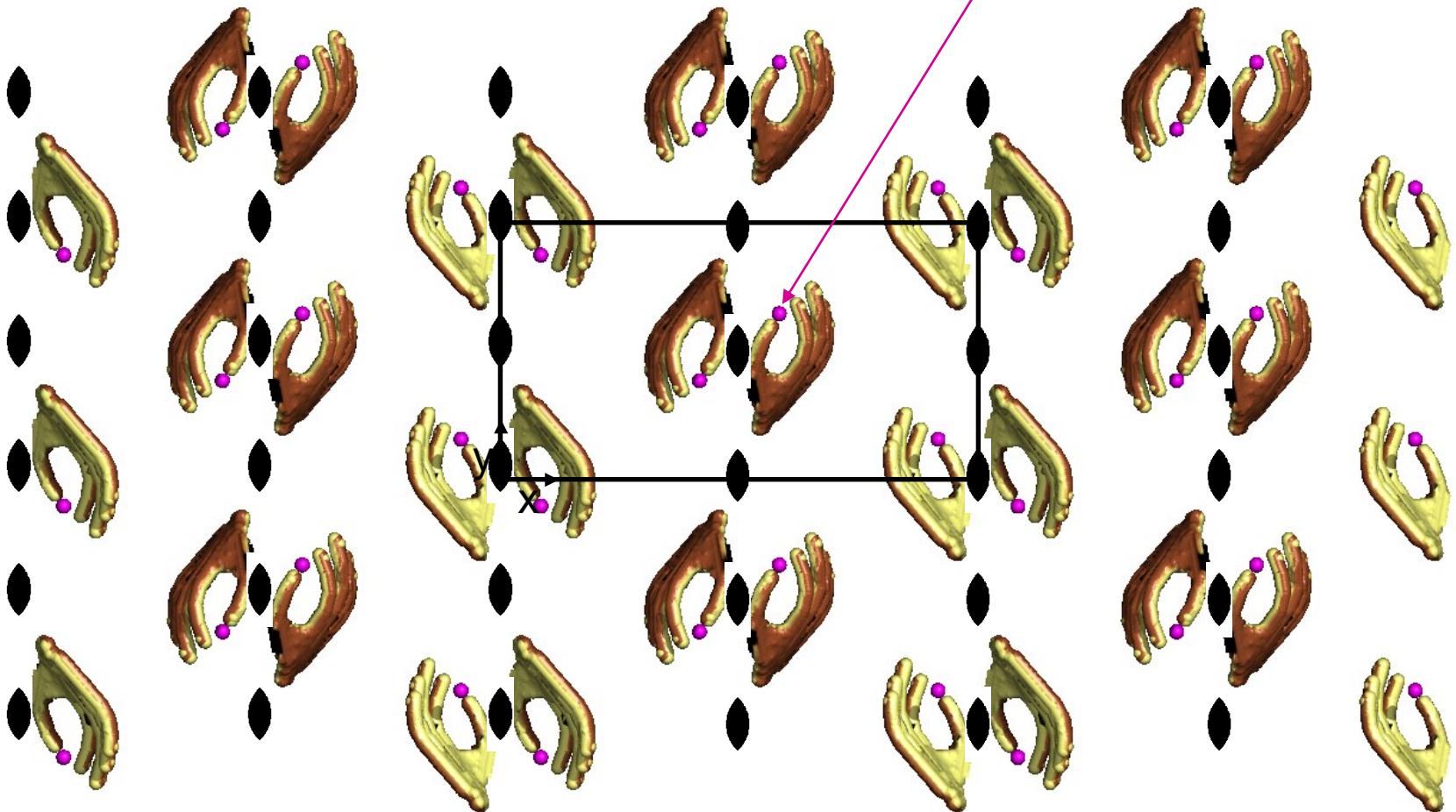
This choice of cell gives

$x=0.084, y=0.633, z=0.075$

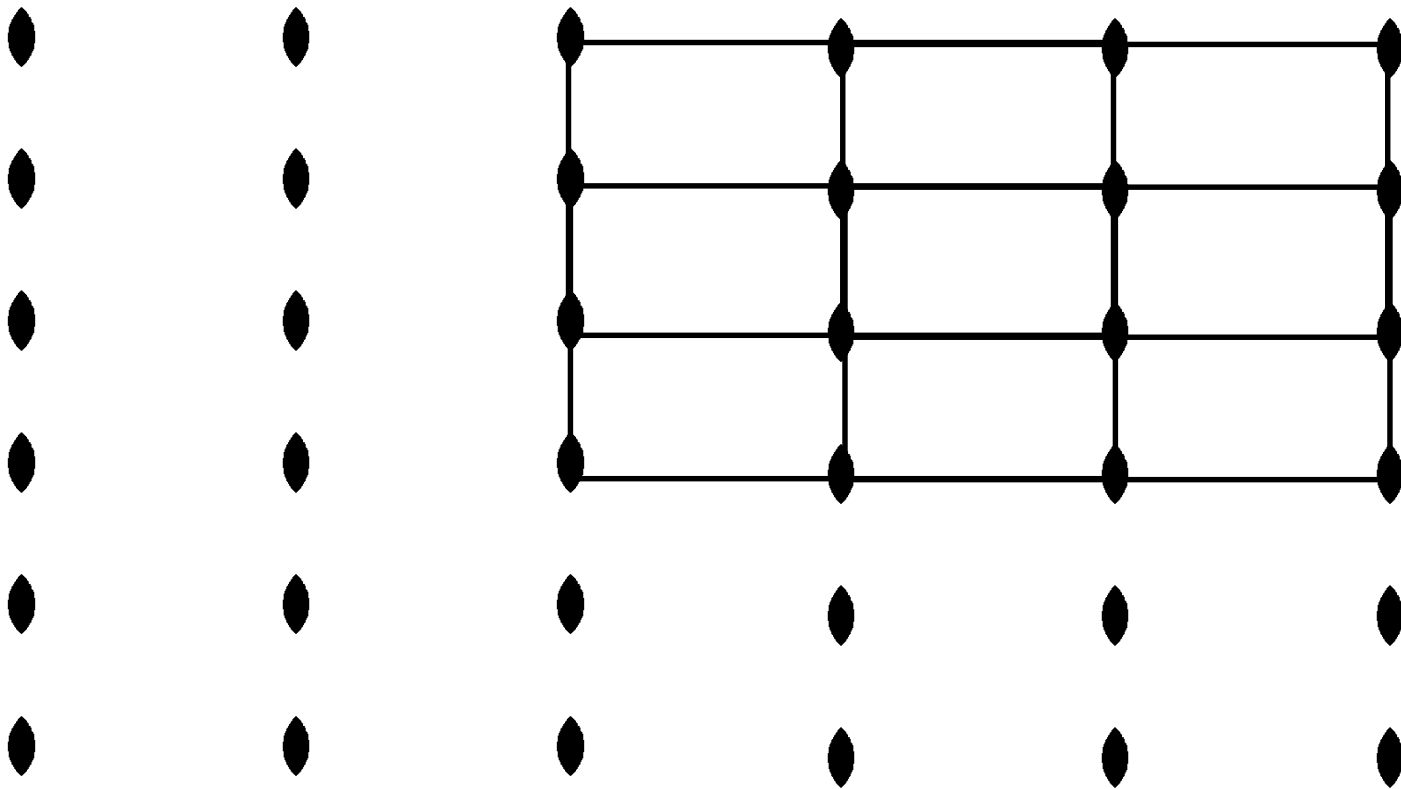


This choice of cell gives

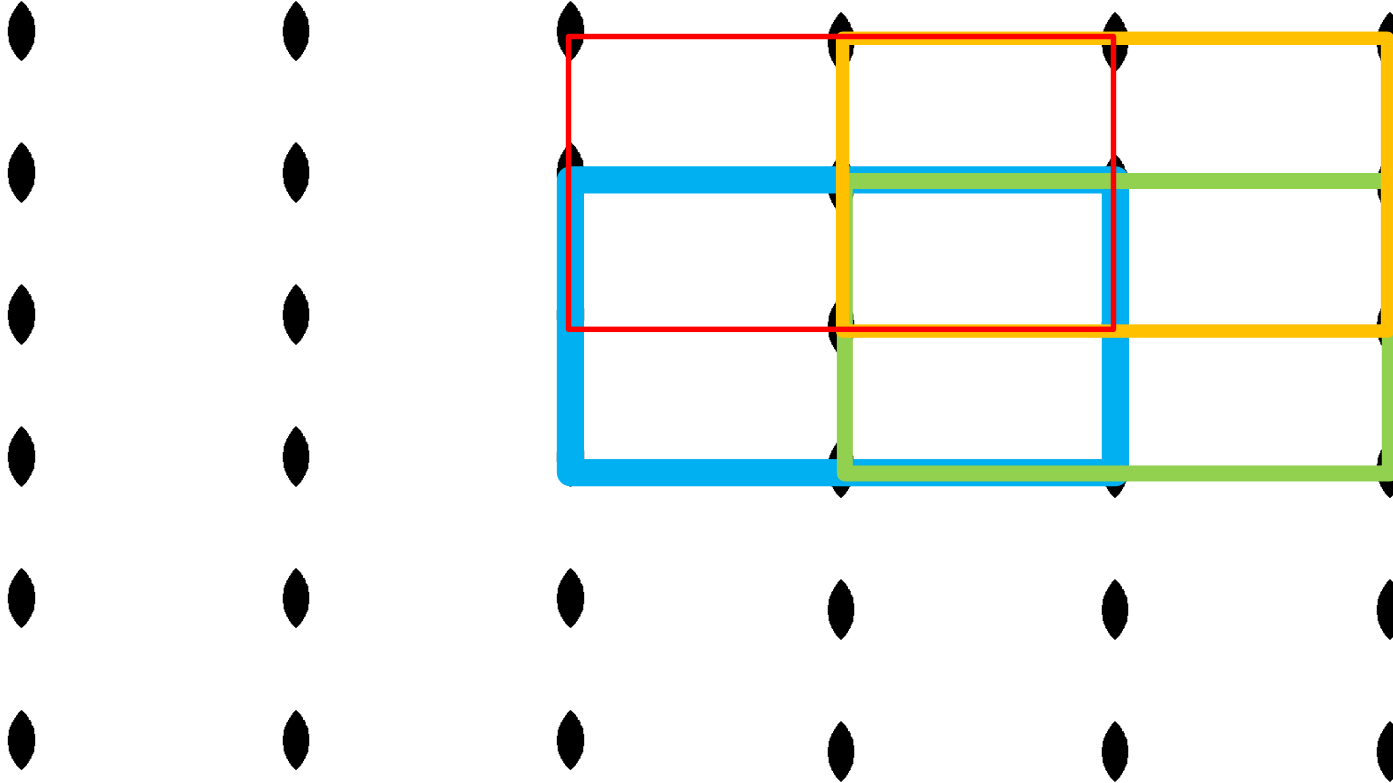
$x=0.584, y=0.633, z=0.075$



There is an ambiguity in the choice of origin



There is an ambiguity in the choice of origin



Cheshire operators

- There are multiple valid numerical values for x, y, z .
- Students with different valid x, y, z will produce maps with identical in features, just shifted in space by a constant.
- The operators that relate valid choices of x, y, z are called Cheshire operators.
- There are 64 Cheshire operators for $P2_12_12$.

Cheshire symmetry allows either choice of x,y,z values

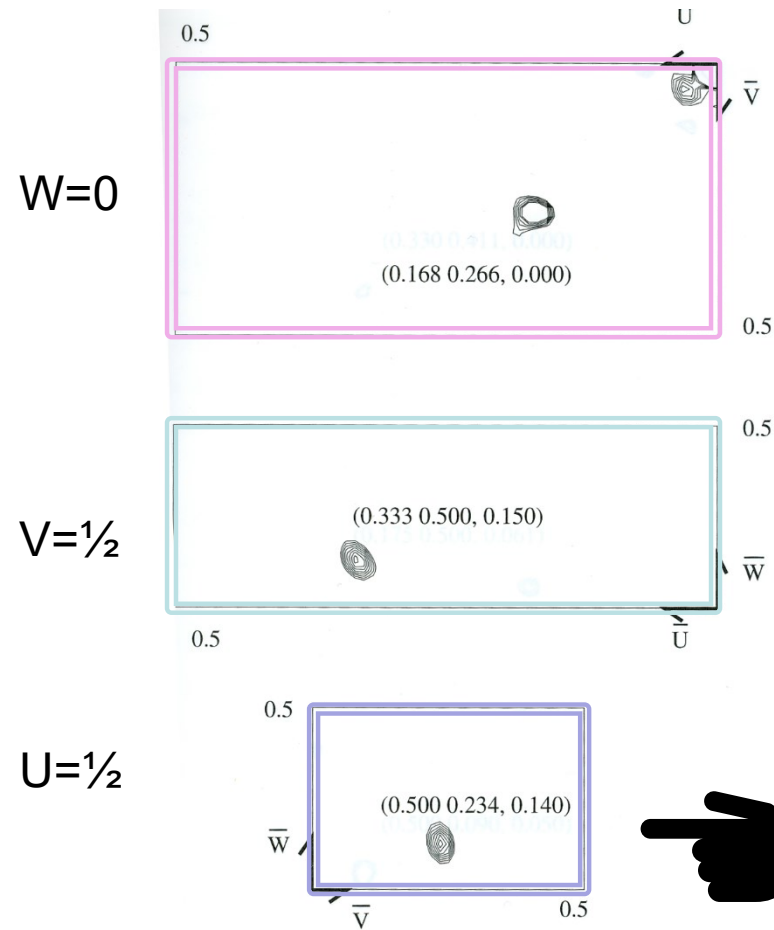
Combo 1 $x_{(\text{from } w=0)}=0.084$, $y_{(\text{from } w=0)}=0.133$, $z_{(\text{from } v=1/2)}=0.075$

Combo 2 $x_{(\text{from } v=1/2)}=0.416$, $y_{(\text{from } w=0)}=0.133$, $z_{(\text{from } v=1/2)}=0.075$

1.	X,	Y,	Z	1) X= 0.084, y= 0.133, z= 0.075	33.	1/2+X, 1/2+Y,	Z	33) X= 0.584, y= 0.633, z= 0.075
2.	-X,	-Y,	Z	2) X=-0.084, y=-0.133, z= 0.075	34.	1/2-X, 1/2-Y,	Z	34) X= 0.416, y= 0.367, z= 0.075
3.	-X,	Y,	-Z	3) X=-0.084, y= 0.133, z=-0.075	35.	1/2-X, 1/2+Y,	-Z	35) X= 0.416, y= 0.633, z=-0.075
4.	X,	-Y,	-Z	4) X= 0.084, y=-0.133, z=-0.075	36.	1/2+X, 1/2-Y,	-Z	36) X= 0.584, y= 0.367, z=-0.075
5.	-X,	-Y,	-Z	5) X=-0.084, y=-0.133, z=-0.075	37.	1/2-X, 1/2-Y,	-Z	37) X= 0.416, y= 0.367, z=-0.075
6.	X,	Y,	-Z	6) X= 0.084, y= 0.133, z=-0.075	38.	1/2+X, 1/2+Y,	-Z	38) X= 0.584, y= 0.633, z=-0.075
7.	X,	-Y,	Z	7) X= 0.084, y=-0.133, z= 0.075	39.	1/2+X, 1/2-Y,	Z	39) X= 0.584, y= 0.367, z= 0.075
8.	-X,	Y,	Z	8) X=-0.084, y= 0.133, z= 0.075	40.	1/2-X, 1/2+Y,	Z	40) X= 0.416, y= 0.633, z= 0.075
9.	1/2+X,	Y,	Z	9) X= 0.584, y= 0.133, z= 0.075	41.	1/2+X,	Y, 1/2+Z	25) X= 0.584, y= 0.133, z= 0.575
10.	1/2-X,	-Y,	Z	10) X= 0.416, y=-0.133, z= 0.075	42.	1/2-X,	-Y, 1/2+Z	26) X= 0.416, y=-0.133, z= 0.575
11.	1/2-X,	Y,	-Z	11) X= 0.416, y= 0.133, z=-0.075	43.	1/2-X,	Y, 1/2-Z	27) X= 0.416, y= 0.133, z= 0.425
12.	1/2+X,	-Y,	-Z	12) X= 0.584, y=-0.133, z=-0.075	44.	1/2+X,	-Y, 1/2-Z	28) X= 0.584, y=-0.133, z= 0.425
13.	1/2-X,	-Y,	-Z	13) X= 0.416, y=-0.133, z=-0.075	45.	1/2-X,	-Y, 1/2-Z	29) X= 0.416, y=-0.133, z= 0.425
14.	1/2+X,	Y,	-Z	14) X= 0.584, y= 0.133, z=-0.075	46.	1/2+X,	Y, 1/2-Z	30) X= 0.584, y= 0.133, z= 0.425
15.	1/2+X,	-Y,	Z	15) X= 0.584, y=-0.133, z= 0.075	47.	1/2+X,	-Y, 1/2+Z	31) X= 0.584, y=-0.133, z= 0.575
16.	1/2-X,	Y,	Z	16) X= 0.416, y= 0.133, z= 0.075	48.	1/2-X,	Y, 1/2+Z	32) X= 0.416, y= 0.133, z= 0.575
17.	X, 1/2+Y,	Z		17) X= 0.084, y= 0.633, z= 0.075	49.	X, 1/2+Y, 1/2+Z		49) X= 0.084, y= 0.633, z= 0.575
18.	-X, 1/2-Y,	Z		18) X=-0.084, y= 0.367, z= 0.075	50.	-X, 1/2-Y, 1/2+Z		50) X=-0.084, y= 0.367, z= 0.575
19.	-X, 1/2+Y,	-Z		19) X=-0.084, y= 0.633, z=-0.075	51.	-X, 1/2+Y, 1/2-Z		51) X=-0.084, y= 0.633, z= 0.425
20.	X, 1/2-Y,	-Z		20) X= 0.084, y= 0.367, z=-0.075	52.	X, 1/2-Y, 1/2-Z		52) X= 0.084, y= 0.367, z= 0.425
21.	-X, 1/2-Y,	-Z		21) X=-0.084, y= 0.367, z=-0.075	53.	-X, 1/2-Y, 1/2-Z		53) X=-0.084, y= 0.367, z= 0.425
22.	X, 1/2+Y,	-Z		22) X= 0.084, y= 0.633, z=-0.075	54.	X, 1/2+Y, 1/2-Z		54) X= 0.084, y= 0.633, z= 0.425
23.	X, 1/2-Y,	Z		23) X= 0.084, y= 0.367, z= 0.075	55.	X, 1/2-Y, 1/2+Z		55) X= 0.084, y= 0.367, z= 0.575
24.	-X, 1/2+Y,	Z		24) X=-0.084, y= 0.633, z= 0.075	56.	-X, 1/2+Y, 1/2+Z		56) X=-0.084, y= 0.633, z= 0.575
25.	X,	Y, 1/2+Z		25) X= 0.084, y= 0.133, z= 0.575	57.	1/2+X, 1/2+Y, 1/2+Z		57) X= 0.584, y= 0.633, z= 0.575
26.	-X,	-Y, 1/2+Z		26) X=-0.084, y=-0.133, z= 0.575	58.	1/2-X, 1/2-Y, 1/2+Z		58) X= 0.416, y= 0.367, z= 0.575
27.	-X,	Y, 1/2-Z		27) X=-0.084, y= 0.133, z= 0.425	59.	1/2-X, 1/2+Y, 1/2-Z		59) X= 0.416, y= 0.633, z= 0.425
28.	X,	-Y, 1/2-Z		28) X= 0.084, y=-0.133, z= 0.425	60.	1/2+X, 1/2-Y, 1/2-Z		60) X= 0.584, y= 0.367, z= 0.425
29.	-X,	-Y, 1/2-Z		29) X=-0.084, y=-0.133, z= 0.425	61.	1/2-X, 1/2-Y, 1/2-Z		61) X= 0.416, y= 0.367, z= 0.425
30.	X,	Y, 1/2-Z		30) X= 0.084, y= 0.133, z= 0.425	62.	1/2+X, 1/2+Y, 1/2-Z		62) X= 0.584, y= 0.633, z= 0.425
31.	X,	-Y, 1/2+Z		31) X= 0.084, y=-0.133, z= 0.575	63.	1/2+X, 1/2-Y, 1/2+Z		63) X= 0.584, y= 0.367, z= 0.575
32.	-X,	Y, 1/2+Z		32) X=-0.084, y= 0.133, z= 0.575	64.	1/2-X, 1/2+Y, 1/2+Z		64) X= 0.416, y= 0.633, z= 0.575

Check your algebra by predicting (u,v,w) of the remaining Patterson peak

Combo 1 $x=0.084, y=0.133, z=0.075$



		1	2	3	4
	Symmetry ops	$x \quad y \quad z$	$-x \quad -y \quad z$	$-x+\frac{1}{2} \quad y+\frac{1}{2} \quad -z$	$x+\frac{1}{2} \quad -y+\frac{1}{2} \quad -z$
1	$x \quad y \quad z$	0 0 0	$-2x \quad -2y \quad 0$	$-2x+\frac{1}{2} \quad \frac{1}{2} \quad -2z$	$\frac{1}{2} \quad -2y+\frac{1}{2} \quad -2z$
2	$-x \quad -y \quad z$	$2x \quad 2y \quad 0$	0 0 0	$\frac{1}{2} \quad 2y+\frac{1}{2} \quad -2z$	$2x+\frac{1}{2} \quad \frac{1}{2} \quad -2z$
3	$-x+\frac{1}{2} \quad y+\frac{1}{2} \quad -z$	$2x-\frac{1}{2} \quad -\frac{1}{2} \quad 2z$	$-1/2 \quad -2y-\frac{1}{2} \quad 2z$	0 0 0	$2x \quad -2y \quad 0$
4	$x+\frac{1}{2} \quad -y+\frac{1}{2} \quad -z$	$-\frac{1}{2} \quad 2y-\frac{1}{2} \quad 2z$	$-2x-\frac{1}{2} \quad -\frac{1}{2} \quad 2z$	$-2x \quad 2y \quad 0$	0 0 0

Plug in values of x,y,z and solve for u,v,w

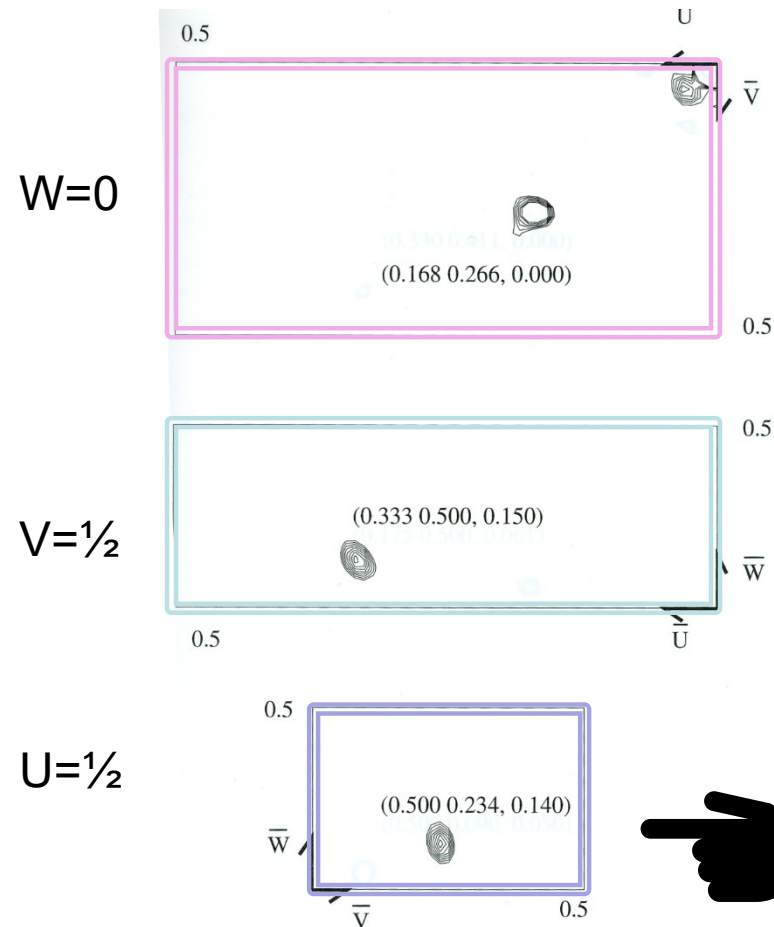
$$U=\frac{1}{2}$$

$$v=-2y+\frac{1}{2}$$

$$w=-2z$$

Check your algebra by predicting (u,v,w) of the remaining Patterson peak

Combo 1 $x=0.084, y=0.133, z=0.075$



		1	2	3	4
	Symmetry ops	$x \quad y \quad z$	$-x \quad -y \quad z$	$-x+\frac{1}{2} \quad y+\frac{1}{2} \quad -z$	$x+\frac{1}{2} \quad -y+\frac{1}{2} \quad -z$
1	$x \quad y \quad z$	0 0 0	$-2x \quad -2y \quad 0$	$-2x+\frac{1}{2} \quad \frac{1}{2} \quad -2z$	$\frac{1}{2} \quad -2y+\frac{1}{2} \quad -2z$
2	$-x \quad -y \quad z$	$2x \quad 2y \quad 0$	0 0 0	$\frac{1}{2} \quad 2y+\frac{1}{2} \quad -2z$	$2x+\frac{1}{2} \quad \frac{1}{2} \quad -2z$
3	$-x+\frac{1}{2} \quad y+\frac{1}{2} \quad -z$	$2x-\frac{1}{2} \quad -\frac{1}{2} \quad 2z$	$-1/2 \quad -2y-\frac{1}{2} \quad 2z$	0 0 0	$2x \quad -2y \quad 0$
4	$x+\frac{1}{2} \quad -y+\frac{1}{2} \quad -z$	$-\frac{1}{2} \quad 2y-\frac{1}{2} \quad 2z$	$-2x-\frac{1}{2} \quad -\frac{1}{2} \quad 2z$	$-2x \quad 2y \quad 0$	0 0 0

$$U=\frac{1}{2}$$

$$\cdot$$

$$\cdot$$

$$U=\frac{1}{2}$$

$$v=-2y+\frac{1}{2}$$

$$v=-2(0.133)+\frac{1}{2}$$

$$v=-0.266+\frac{1}{2}$$

$$\mathbf{v=0.234}$$

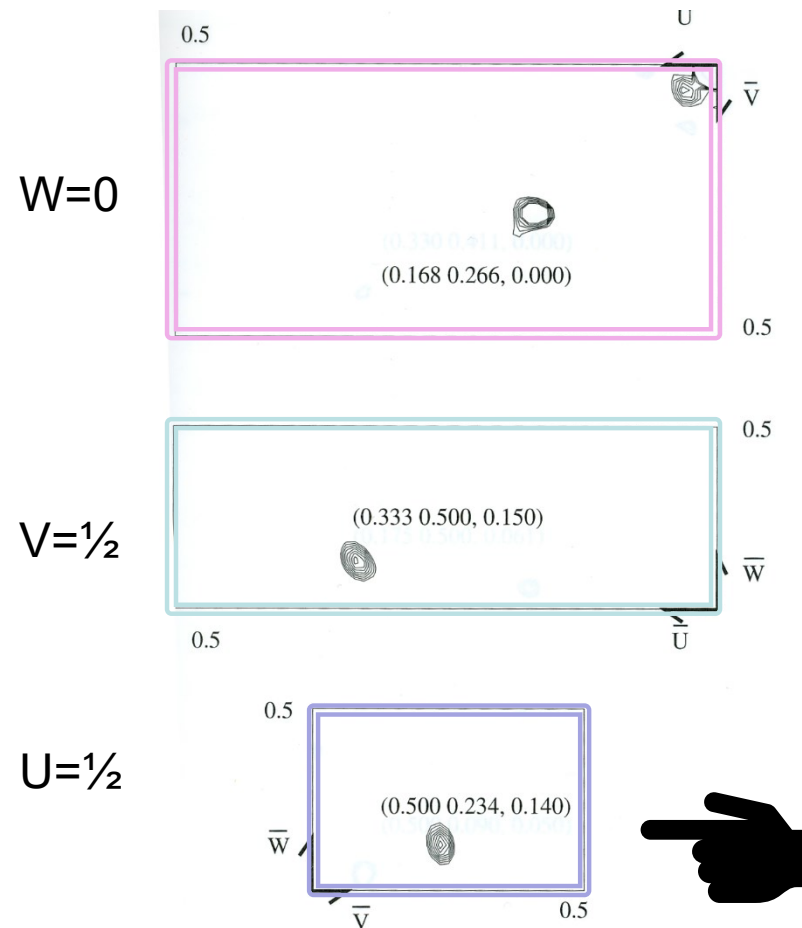
$$w=-2z$$

$$\cdot$$

$$w=-2(0.075)$$

$$\mathbf{w=-0.140}$$

Is the prediction ($\frac{1}{2}, 0.234, -0.140$) a match with recorded peak ($\frac{1}{2}, 0.234, 0.140$)?



Patterson symmetry operators for $P2_12_12$ (Pmmm)

U, V, W
 $-U, -V, W$
 $-U, V, -W$
 $U, -V, -W$
 $-U, -V, -W$
 $U, V, -W$
 $U, -V, W$
 $-U, V, W$

$U=\frac{1}{2}$
 $\cdot$
 $\cdot$
 $U=\frac{1}{2}$

$v=-2y+\frac{1}{2}$
 $v=-2(0.133)+\frac{1}{2}$
 $v=-0.266+\frac{1}{2}$
 $v=0.234$

$w=-2z$
 $w=-2(0.075)$
 $w=-0.140$

Yes, by Patterson symmetry operator **$u, v, -w$** we confirm that ($u=\frac{1}{2}, v=0.234, w=-0.140$) equals ($u=\frac{1}{2}, v=0.234, w=0.140$)

Congratulations!

- You successfully determined the heavy atom substructure for this Pt derivative of DNA polymerase β .

$$x=0.084, y=0.133, z=0.075$$

- Now, you are ready to calculate phases and then a map, and this will reveal shape of the protein.

Advanced case, Proteinase K in space group $P4_32_12$

- How many Patterson peaks?
- Where are Harker sections?

$P4_32_12$

No. 96

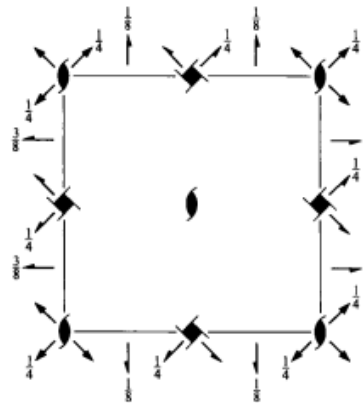
D_4^8

$P4_32_12$

422

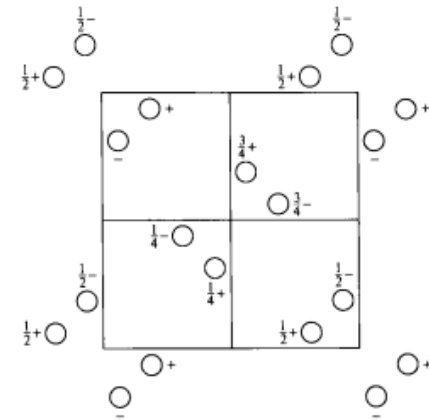
Tetragonal

Patterson symmetry $P4/mmm$



Origin on $2[110]$ at $2_1(1,2)$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$



1 x, y, z

2 $\bar{x}, \bar{y}, \frac{1}{2} + z$

3 $\frac{1}{2} - y, \frac{1}{2} + x, \frac{3}{4} + z$

4 $\frac{1}{2} + y, \frac{1}{2} - x, \frac{1}{4} + z$

5 $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{4} - z$

6 $\frac{1}{2} - x, \frac{1}{2} + y, \frac{3}{4} - z$

7 $\bar{y}, \bar{x}, \frac{1}{2} - z$

8 $y, x, \bar{z}$

$8 \times 8 = 64$ Patterson peaks

8 peaks are located at the origin

$64 - 8 = 56$ non-origin peaks

$56 / 2 = 28$ peaks are related to the remaining 28 peaks by center of inversion

28 unique Patterson peaks are expected

1)	x	y	z
2)	-x	-y	1/2+z
	2x	2y	-1/2

Table of Patterson Difference Vectors (U,V,W)

1)	x	y	z
3)	1/2-y	1/2+x	3/4+z
	-1/2+x+y	-1/2-x+y	-3/4

2)	-x	-y	1/2+z
3)	1/2-y	1/2+x	3/4+z
	-1/2-x+y	-1/2-x-y	-1/4

1)	x	y	z
4)	1/2+y	1/2-x	1/4+z
	-1/2+x-y	-1/2+x+y	-1/4

2)	-x	-y	1/2+z
4)	1/2+y	1/2-x	1/4+z
	-1/2-x-y	-1/2+x-y	1/4

3)	1/2-y	1/2+x	3/4+z
4)	1/2+y	1/2-x	1/4+z
	-2y	2x	1/2

8 symmetry operators in
space group $P4_32_12$

1)	x	y	z
2)	-x	-y	1/2+z
3)	1/2-y	1/2+x	3/4+z
4)	1/2+y	1/2-x	1/4+z
5)	y	x	-z
6)	-y	-x	1/2-z
7)	1/2-x	1/2+y	3/4-z
8)	1/2+x	1/2-y	1/4-z

1)	x	y	z
5)	y	x	-z
	x-y	-x+y	2z

2)	-x	-y	1/2+z
5)	y	x	-z
	-x-y	-x-y	1/2+2z

3)	1/2-y	1/2+x	3/4+z
5)	y	x	-z
	1/2-2y	1/2	3/4+2z

4)	1/2+y	1/2-x	1/4+z
5)	y	x	-z
	1/2	1/2-2x	1/4+2z

7)	1/2-x	1/2+y	3/4-z
8)	1/2+x	1/2-y	1/4-z
	-2x	2y	1/2

1)	x	y	z
6)	-y	-x	1/2-z
	x+y	x+y	-1/2+2z

2)	-x	-y	1/2+z
6)	-y	-x	1/2-z
	-x+y	x-y	2z

3)	1/2-y	1/2+x	3/4+z
6)	-y	-x	1/2-z
	1/2	1/2+2x	1/4+2z

4)	1/2+y	1/2-x	1/4+z
6)	-y	-x	1/2-z
	1/2+2y	1/2	-1/4+2z

5)	y	x	-z
6)	-y	-x	1/2-z
	2y	2x	-1/2

1)	x	y	z
7)	1/2-x	1/2+y	3/4-z
	-1/2+2x	-1/2	-3/4+2z

2)	-x	-y	1/2+z
7)	1/2-x	1/2+y	3/4-z
	-1/2	-1/2-2y	-1/4+2z

3)	1/2-y	1/2+x	3/4+z
7)	1/2-x	1/2+y	3/4-z
	x-y	x-y	2z

4)	1/2+y	1/2-x	1/4+z
7)	1/2-x	1/2+y	3/4-z
	x+y	-x-y	-1/2+2z

5)	y	x	-z
7)	1/2-x	1/2+y	3/4-z
	-1/2+x+y	-1/2+x-y	-3/4

6)	-y	-x	1/2-z
7)	1/2-x	1/2+y	3/4-z
	-1/2-x-y	-1/2-x-y	-1/4

1)	x	y	z
8)	1/2+x	1/2-y	1/4-z
	-1/2	-1/2+2y	-1/4+2z

2)	-x	-y	1/2+z
8)	1/2+x	1/2-y	1/4-z
	-1/2-2x	-1/2	1/4+2z

3)	1/2-y	1/2+x	3/4+z
8)	1/2+x	1/2-y	1/4-z
	-x-y	x+y	1/2+2z

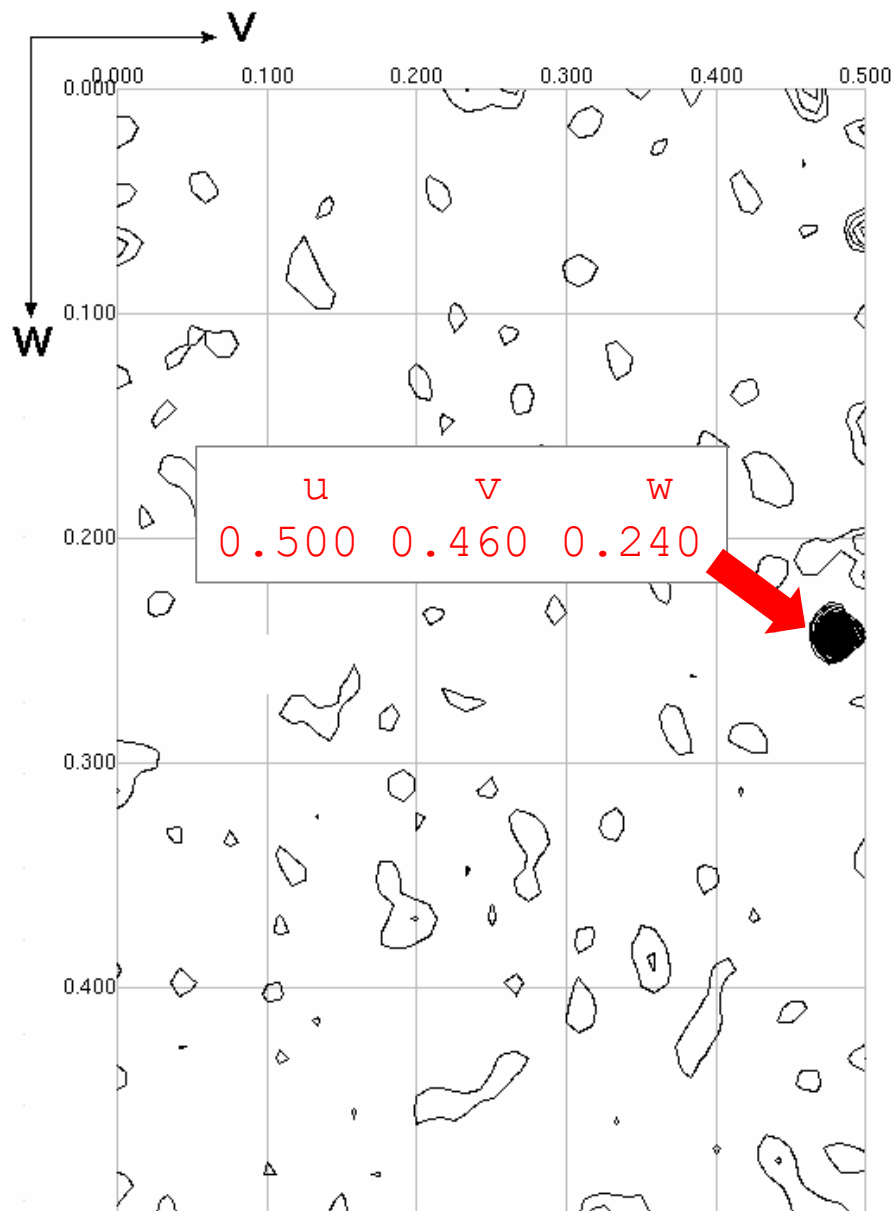
4)	1/2+y	1/2-x	1/4+z
8)	1/2+x	1/2-y	1/4-z
	-x+y	-x+y	2z

5)	y	x	-z
8)	1/2+x	1/2-y	1/4-z
	-1/2-x+y	-1/2+x+y	-1/4

6)	-y	-x	1/2-z
8)	1/2+x	1/2-y	1/4-z
	-1/2-x-y	-1/2-x-y	1/4

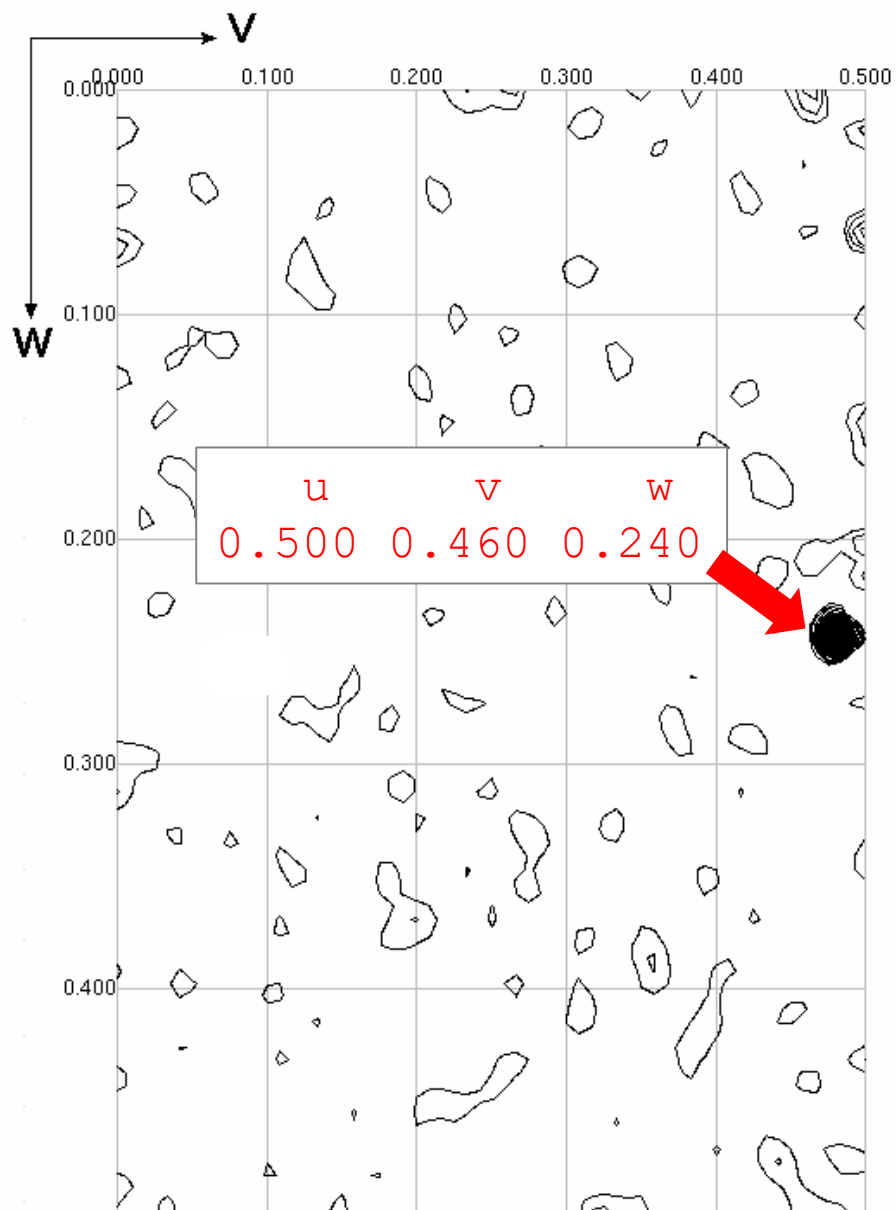
isomorphous difference Patterson map

$u=0.50$



isomorphous difference Patterson map

$u=0.50$



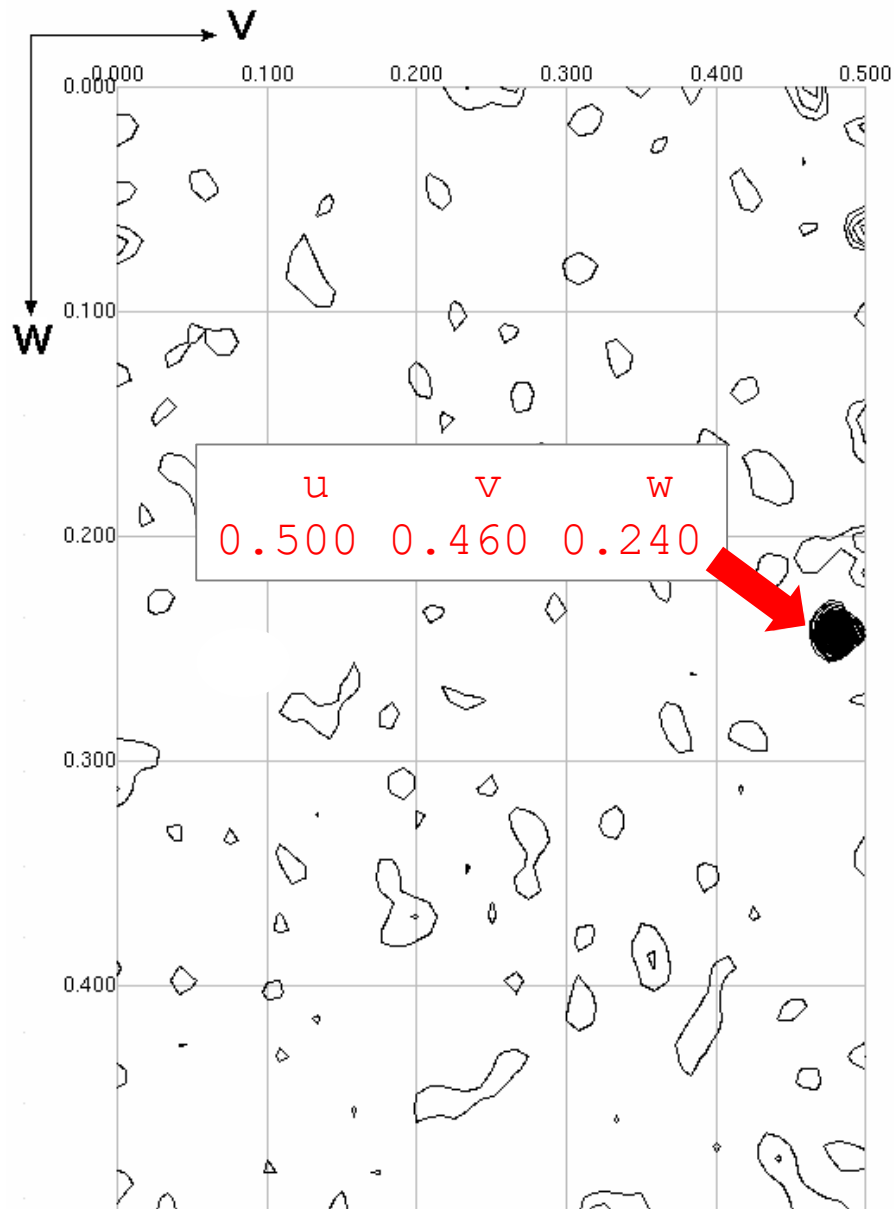
Symmetry operator 3

-Symmetry operator 6

$\frac{1}{2}-y$	$\frac{1}{2}+x$	$\frac{3}{4}+z$
$-(-y$	$-x$	$\frac{1}{2}-z)$
$u=\frac{1}{2},$	$v=\frac{1}{2}+2x,$	$w=\frac{1}{4}+2z$

isomorphous difference Patterson map

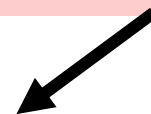
$u=0.50$



Symmetry operator 3

-Symmetry operator 6

$$\begin{array}{ccc} \frac{1}{2}-y & \frac{1}{2}+x & \frac{3}{4}+z \\ -(-y) & -x & \frac{1}{2}-z \end{array} \quad \begin{array}{l} u=\frac{1}{2}, \\ v=\frac{1}{2}+2x, \\ w=\frac{1}{4}+2z \end{array}$$

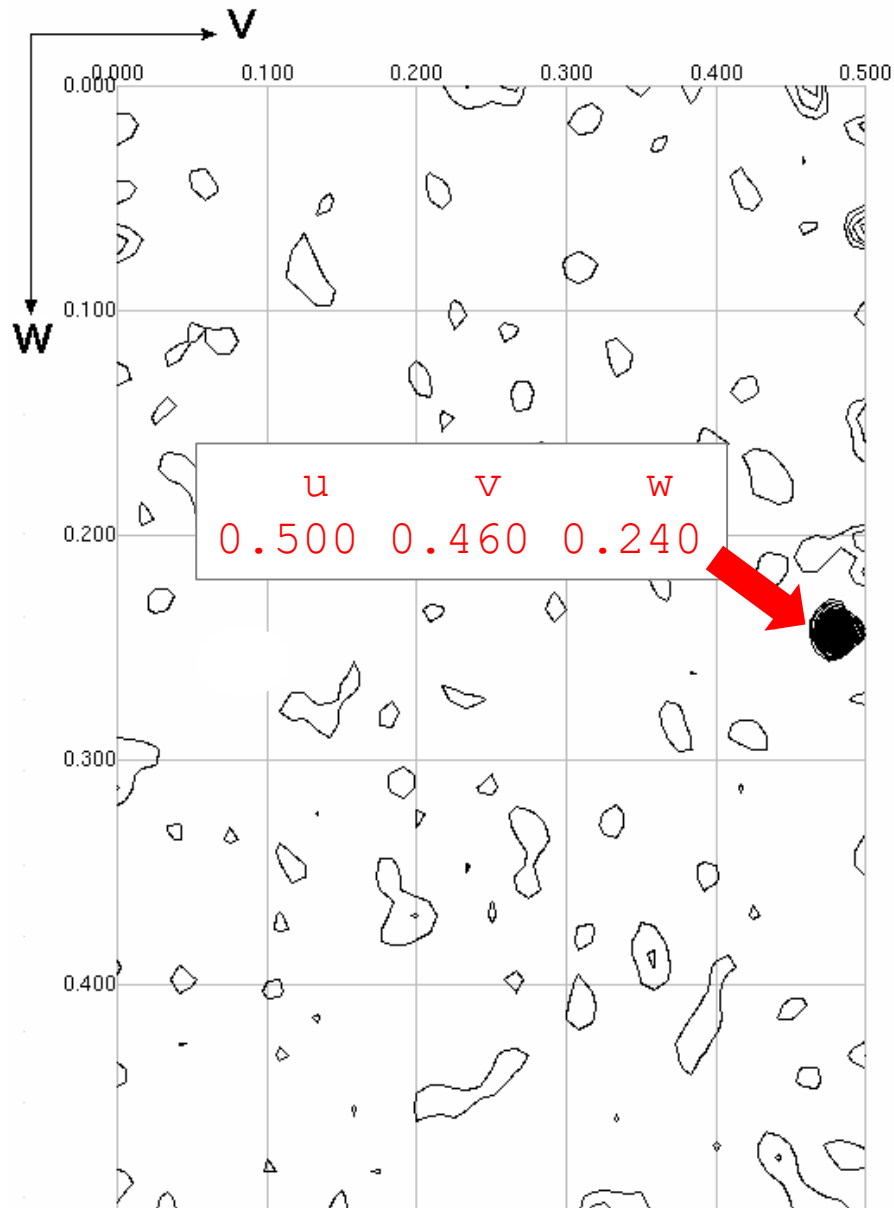


Plug in v ,
solve for x :

$$\begin{aligned} v &= \frac{1}{2} + 2x \\ 0.460 &= \frac{1}{2} + 2x \\ -0.040 &= 2x \\ -0.020 &= x \end{aligned}$$

isomorphous difference Patterson map

$u=0.50$



Symmetry operator 3

-Symmetry operator 6

$$\begin{array}{ccc} \frac{1}{2}-y & \frac{1}{2}+x & \frac{3}{4}+z \\ -(-y) & -x & \frac{1}{2}-z \\ \hline u=\frac{1}{2}, & v=\frac{1}{2}+2x, & w=\frac{1}{4}+2z \end{array}$$

Plug in v ,
solve for x :

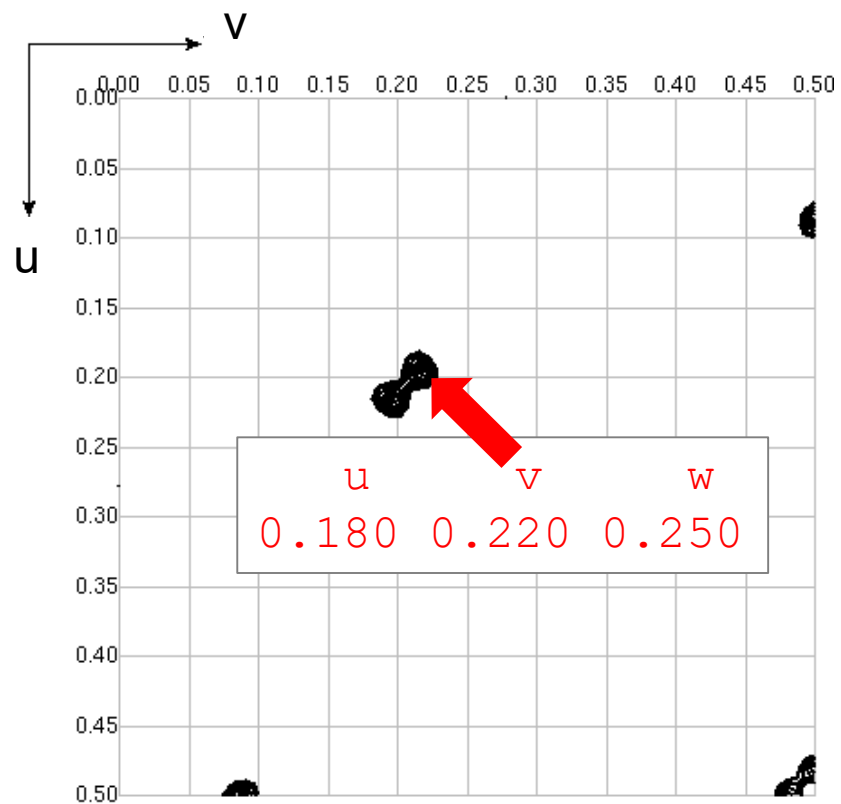
$$\begin{aligned} v &= \frac{1}{2} + 2x \\ 0.460 &= \frac{1}{2} + 2x \\ -0.040 &= 2x \\ -0.020 &= x \end{aligned}$$

Plug in w ,
solve for z :

$$\begin{aligned} w &= \frac{1}{4} + 2z \\ 0.240 &= \frac{1}{4} + 2z \\ -0.010 &= 2z \\ -0.005 &= z \end{aligned}$$

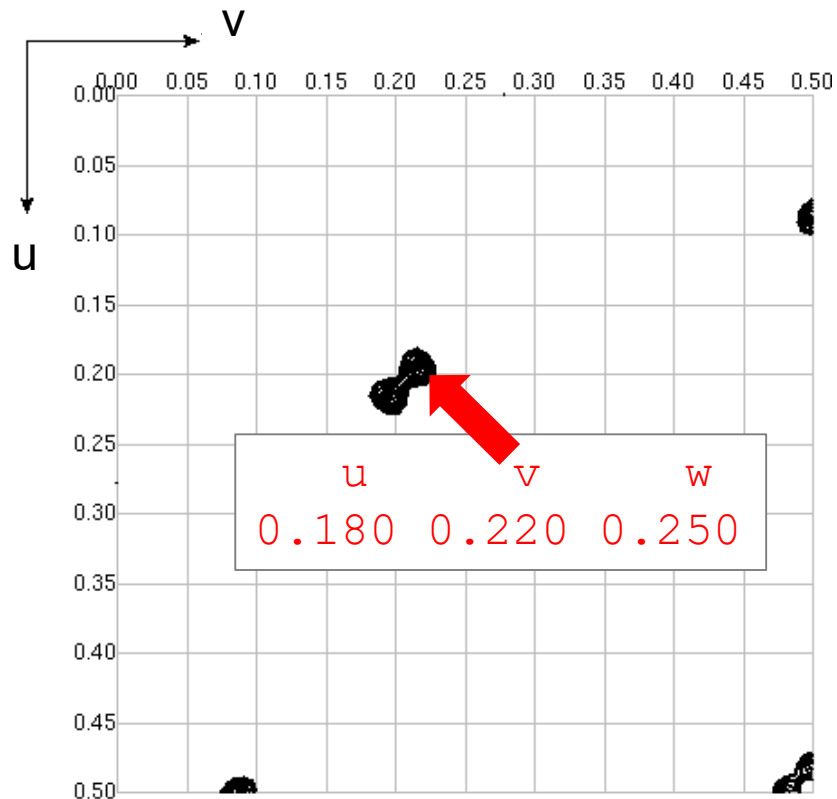
isomorphous difference Patterson map

$W=0.25$



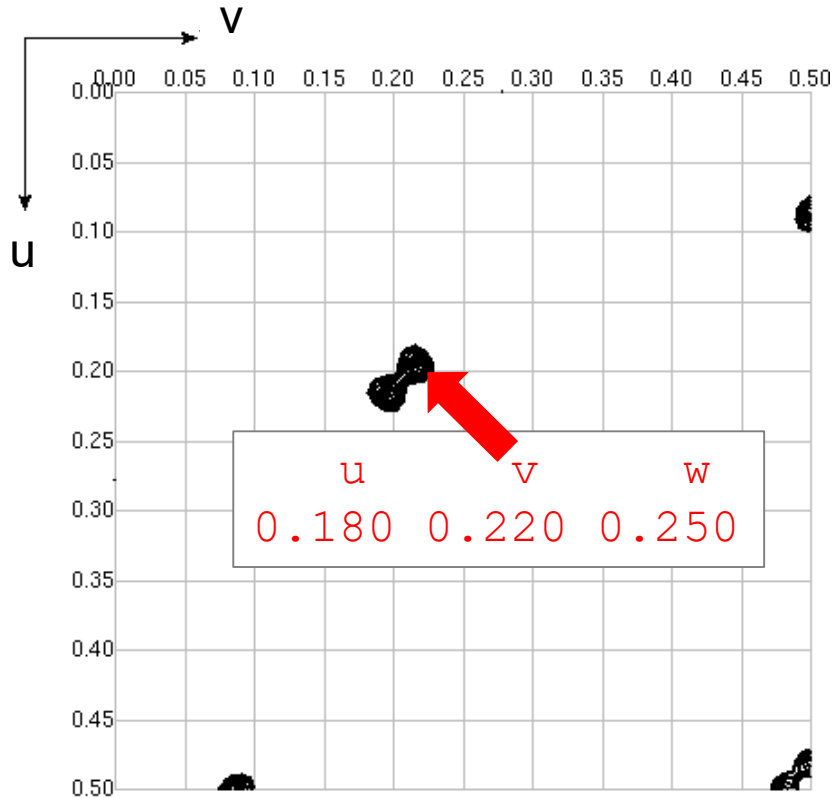
Symmetry operator 2 -Symmetry operator 4

isomorphous difference Patterson map
W=0.25



2)	$-x$	$-y$	$\frac{1}{2}+z$
4)	$-(\frac{1}{2}+y)$	$\frac{1}{2}-x$	$\frac{1}{4}+z$
$u=-\frac{1}{2}-x-y, \quad v=-\frac{1}{2}+x-y, \quad w=\frac{1}{4}$			

isomorphous difference Patterson map
 $W=0.25$



Symmetry operator 2
 -Symmetry operator 4

2)	$-x$	$-y$	$\frac{1}{2}+z$
4)	$-(\frac{1}{2}+y)$	$\frac{1}{2}-x$	$\frac{1}{4}+z$
$u=-\frac{1}{2}-x-y, \quad v=-\frac{1}{2}+x-y, \quad w=\frac{1}{4}$			



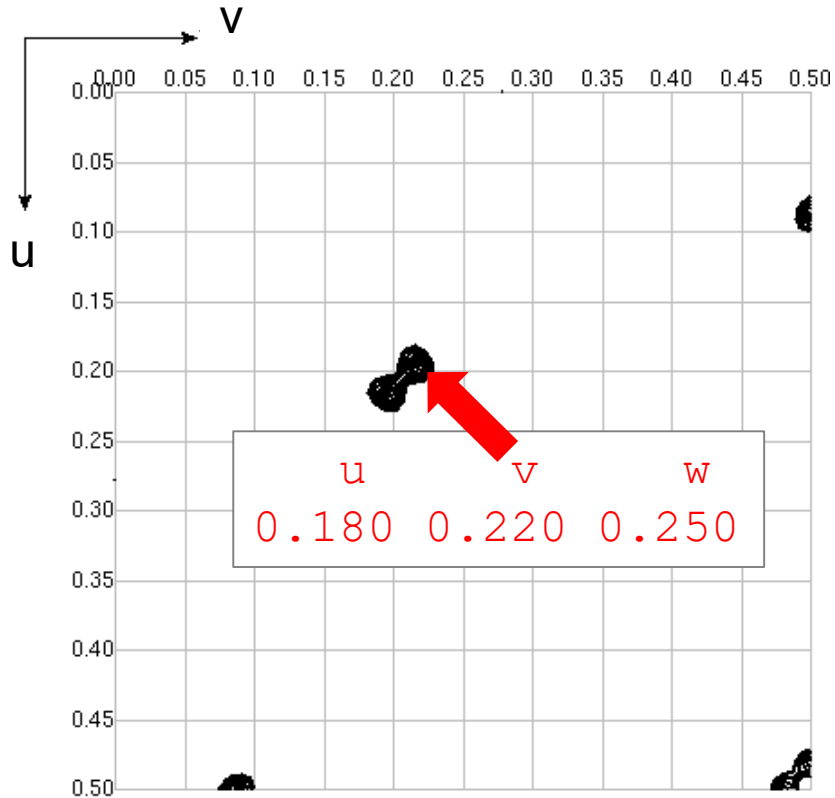
Plug in u and
 solve for x.

$$u = -\frac{1}{2} - x - y$$

$$0.180 = -\frac{1}{2} - x - y$$

$$0.680 = -x - y$$

isomorphous difference Patterson map
 $W=0.25$



Symmetry operator 2
 -Symmetry operator 4

2)	$-x$	$-y$	$\frac{1}{2}+z$
4)	$-(\frac{1}{2}+y)$	$\frac{1}{2}-x$	$\frac{1}{4}+z$
$u=-\frac{1}{2}-x-y, \quad v=-\frac{1}{2}+x-y, \quad w=\frac{1}{4}$			

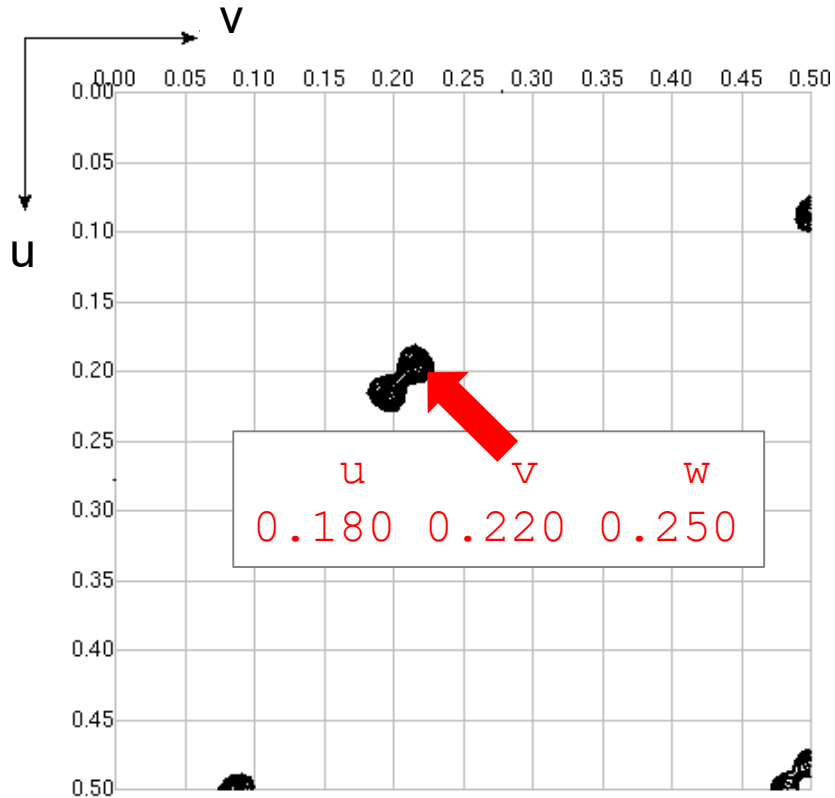
Plug in u and
 solve for x.

$$\begin{aligned} u &= -\frac{1}{2} - x - y \\ 0.180 &= -\frac{1}{2} - x - y \\ 0.680 &= -x - y \end{aligned}$$

Plug in v and
 solve for y.

$$\begin{aligned} v &= -\frac{1}{2} + x - y \\ 0.220 &= -\frac{1}{2} + x - y \\ 0.720 &= x - y \end{aligned}$$

isomorphous difference Patterson map
 $W=0.25$



Symmetry operator 2
 -Symmetry operator 4

2)	$-x$	$-y$	$\frac{1}{2}+z$
4)	$-(\frac{1}{2}+y)$	$\frac{1}{2}-x$	$\frac{1}{4}+z$
$u=-\frac{1}{2}-x-y, \quad v=-\frac{1}{2}+x-y, \quad w=\frac{1}{4}$			

Plug in u and
 solve for x.

$$\begin{aligned} u &= -\frac{1}{2} - x - y \\ 0.180 &= -\frac{1}{2} - x - y \\ 0.680 &= -x - y \end{aligned}$$

Subtract equations

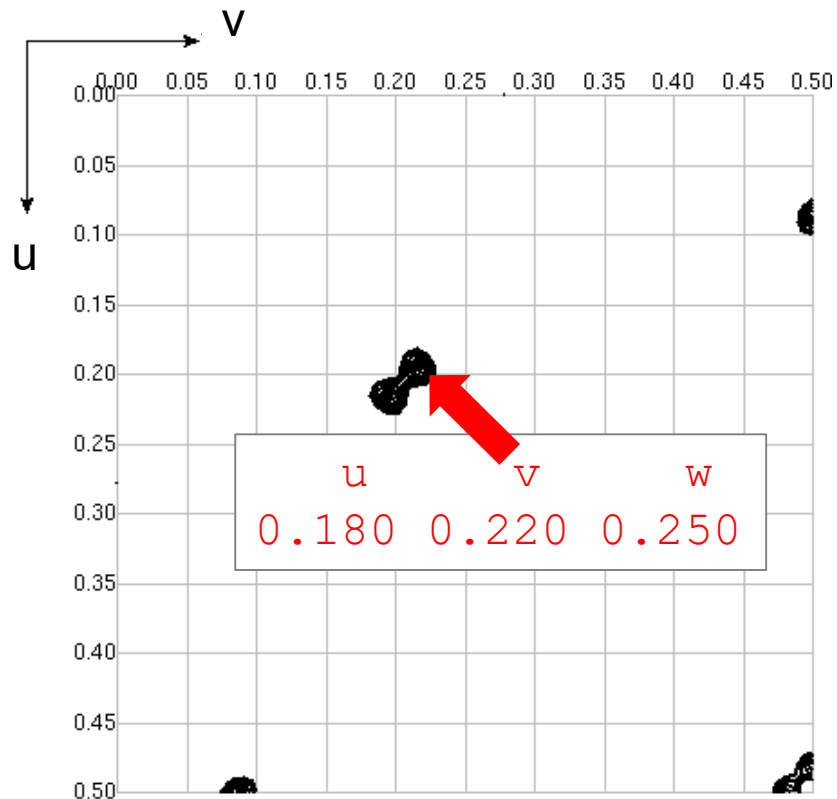
$$\begin{aligned} 0.680 &= -x - y \\ -0.720 &= -x + y \\ \hline -0.040 &= -2x \end{aligned}$$

$$0.020 = x$$

Plug in v and
 solve for y.

$$\begin{aligned} v &= -\frac{1}{2} + x - y \\ 0.220 &= -\frac{1}{2} + x - y \\ 0.720 &= x - y \end{aligned}$$

isomorphous difference Patterson map
W=0.25



Symmetry operator 2
-Symmetry operator 4

2)	$-x$	$-y$	$\frac{1}{2}+z$
4)	$-(\frac{1}{2}+y)$	$\frac{1}{2}-x$	$\frac{1}{4}+z$
$u = -\frac{1}{2}-x-y, \quad v = -\frac{1}{2}+x-y, \quad w = \frac{1}{4}$			

Plug in u and
solve for x.

$$\begin{aligned} u &= -\frac{1}{2} - x - y \\ 0.180 &= -\frac{1}{2} - x - y \\ 0.680 &= -x - y \end{aligned}$$

Subtract equations

$$\begin{aligned} 0.680 &= -x - y \\ -0.720 &= -x + y \\ \hline -0.040 &= -2x \end{aligned}$$

$$0.020 = x$$

Plug in v and
solve for y.

$$\begin{aligned} v &= -\frac{1}{2} + x - y \\ 0.220 &= -\frac{1}{2} + x - y \\ 0.720 &= x - y \end{aligned}$$

Add equations

$$\begin{aligned} 0.720 &= x - y \\ 0.680 &= -x - y \\ \hline 1.400 &= -2y \end{aligned}$$

$$-0.700 = y$$

How to merge atom coordinates x, y, and z from two Harker sections

From Harker section $u=\frac{1}{2}$ we get: $X_1 = \underline{-0.020}$ $Y_1 = \underline{\hspace{1cm}}$ $z_1 = \underline{-0.005}$

From Harker section $w=\frac{1}{4}$ we get: $X_2 = \underline{+0.020}$ $Y_2 = \underline{-0.700}$ $z_2 = \underline{\hspace{1cm}}$

- Note x_1 and x_2 are unequal: $-0.020 \neq +0.020$.
- Both coordinate sets are correct; they describe different atoms in the unit cell (related by $P4_32_12$ symmetry) or different origin choices.
- Sadly, both coordinate sets are incomplete; y_1 and z_2 are unknown.

How to merge atom coordinates x, y, and z from two Harker sections

From Harker section $u=\frac{1}{2}$ we get: $X_1 = \underline{-0.020}$ $y_1 = \underline{\hspace{1cm}}$ $z_1 = \underline{-0.005}$

From Harker section $w=\frac{1}{4}$ we get: $X_2 = \underline{+0.020}$ $y_2 = \underline{-0.700}$ $z_2 = \underline{\hspace{1cm}}$

- We must combine coordinates (x_1, z_1) and (x_2, y_2) to get a complete triplet: either (x_1, y_1, z_1) or (x_2, y_2, z_2) .
- Search for a Cheshire operator that relates (x_1, y_1, z_1) to (x_2, y_2, z_2)
 - In this case, we need a Cheshire operator that negates x
 - (i.e. transforms $x_2 = 0.020$ to $x_1 = -0.020$).
- Apply this Cheshire operator to (x_2, y_2, z_2) to get value of y_1 , completing the set (x_1, y_1, z_1) .

From Harker section $u=1/2$

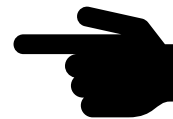
$$X_1 = \underline{-0.020}, \quad y_1 = \underline{\hspace{1cm}}, \quad z_1 = \underline{-0.005}$$

From Harker section $w=1/4$

$$X_2 = \underline{+0.020}, \quad y_2 = \underline{-0.700}, \quad z_2 = \underline{\hspace{1cm}}$$

Cheshire Symmetry Operators for space group $P4_32_12$

1	X,	Y,	Z
2	-X,	-Y,	Z
3	-Y,	X,	1/4+Z
4	Y,	-X,	1/4+Z
5	Y,	X,	-Z
6	-Y,	-X,	-Z
7	X,	-Y,	1/4-Z
8	-X,	Y,	1/4-Z



This operator
will do what we
want: negate x

09	1/2+X,	1/2+Y,	Z
10	1/2-X,	1/2-Y,	Z
11	1/2-Y,	1/2+X,	1/4+Z
12	1/2+Y,	1/2-X,	1/4+Z
13	1/2+Y,	1/2+X,	-Z
14	1/2-Y,	1/2-X,	-Z
15	1/2+X,	1/2-Y,	1/4-Z
16	1/2-X,	1/2+Y,	1/4-Z

17	X,	Y,	1/2+Z
18	-X,	-Y,	1/2+Z
19	-Y,	X,	3/4+Z
20	Y,	-X,	3/4+Z
21	Y,	X,	1/2-Z
22	-Y,	-X,	1/2-Z
23	X,	-Y,	3/4-Z
24	-X,	Y,	3/4-Z

25	1/2+X,	1/2+Y,	1/2+Z
26	1/2-X,	1/2-Y,	1/2+Z
27	1/2-Y,	1/2+X,	3/4+Z
28	1/2+Y,	1/2-X,	3/4+Z
29	1/2+Y,	1/2+X,	1/2-Z
30	1/2-Y,	1/2-X,	1/2-Z
31	1/2+X,	1/2-Y,	3/4-Z
32	1/2-X,	1/2+Y,	3/4-Z

From Harker section $u=1/2$

$$X_1 = \underline{-0.020}, \quad y_1 = \underline{\hspace{1cm}}, \quad z_1 = \underline{-0.005}$$

From Harker section $w=1/4$

$$X_2 = \underline{+0.020}, \quad y_2 = \underline{-0.700}, \quad z_2 = \underline{\hspace{1cm}}$$

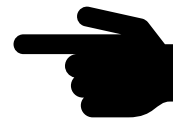
-x, -y, z

Apply Cheshire operator (2)

$$X_2 = \underline{-0.020}, \quad y_2 = \underline{+0.700}, \quad z_2 = \underline{\hspace{1cm}}$$

Cheshire Symmetry Operators for space group $P4_32_12$

1	X,	Y,	Z
2	-x,	-y,	z
3	-Y,	X,	1/4+Z
4	Y,	-X,	1/4+Z
5	Y,	X,	-Z
6	-Y,	-X,	-Z
7	X,	-Y,	1/4-Z
8	-X,	Y,	1/4-Z



This operator
will do what we
want: negate x

09	1/2+X,	1/2+Y,	Z
10	1/2-X,	1/2-Y,	Z
11	1/2-Y,	1/2+X,	1/4+Z
12	1/2+Y,	1/2-X,	1/4+Z
13	1/2+Y,	1/2+X,	-Z
14	1/2-Y,	1/2-X,	-Z
15	1/2+X,	1/2-Y,	1/4-Z
16	1/2-X,	1/2+Y,	1/4-Z

17	X,	Y,	1/2+Z
18	-X,	-Y,	1/2+Z
19	-Y,	X,	3/4+Z
20	Y,	-X,	3/4+Z
21	Y,	X,	1/2-Z
22	-Y,	-X,	1/2-Z
23	X,	-Y,	3/4-Z
24	-X,	Y,	3/4-Z

25	1/2+X,	1/2+Y,	1/2+Z
26	1/2-X,	1/2-Y,	1/2+Z
27	1/2-Y,	1/2+X,	3/4+Z
28	1/2+Y,	1/2-X,	3/4+Z
29	1/2+Y,	1/2+X,	1/2-Z
30	1/2-Y,	1/2-X,	1/2-Z
31	1/2+X,	1/2-Y,	3/4-Z
32	1/2-X,	1/2+Y,	3/4-Z

From Harker section $u=1/2$

$$X_1 = \underline{-0.020}, \quad y_1 = \underline{\hspace{1cm}}, \quad z_1 = \underline{-0.005}$$

From Harker section $w=1/4$

$$X_2 = \underline{+0.020}, \quad y_2 = \underline{-0.700}, \quad z_2 = \underline{\hspace{1cm}}$$

-x, -y, z

Apply Cheshire operator (2)

$$X_2 = \underline{-0.020}, \quad y_2 = \underline{+0.700}, \quad z_2 = \underline{\hspace{1cm}}$$

Now, we can merge x_2, y_2, z_2 with x_1, y_1, z_1
Arriving at complete heavy atom coordinate set:

$$x_1 = -0.020, \quad y_1 = +0.700, \quad z_1 = -0.005$$

Cheshire Symmetry Operators for space group $P4_32_12$

1	X,	Y,	Z
2	-x,	-y,	z
3	-Y,	X,	1/4+Z
4	Y,	-X,	1/4+Z
5	Y,	X,	-Z
6	-Y,	-X,	-Z
7	X,	-Y,	1/4-Z
8	-X,	Y,	1/4-Z



This operator
will do what we
want: negate x

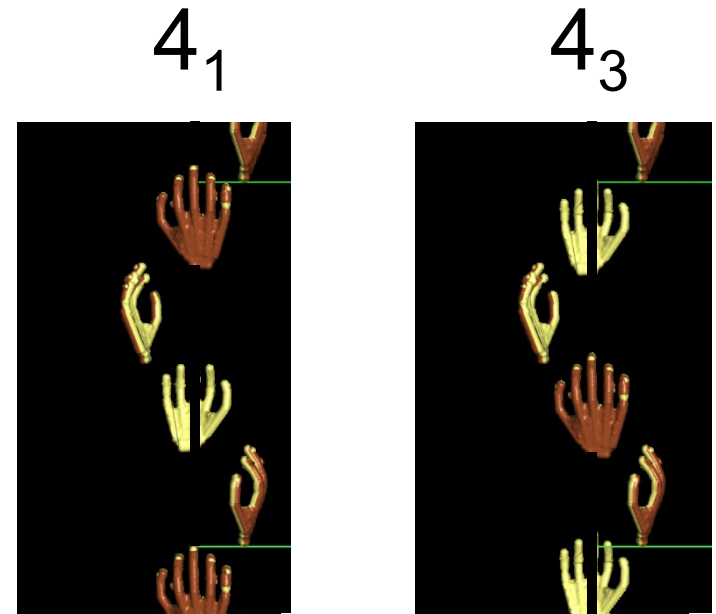
09	1/2+X,	1/2+Y,	Z
10	1/2-X,	1/2-Y,	Z
11	1/2-Y,	1/2+X,	1/4+Z
12	1/2+Y,	1/2-X,	1/4+Z
13	1/2+Y,	1/2+X,	-Z
14	1/2-Y,	1/2-X,	-Z
15	1/2+X,	1/2-Y,	1/4-Z
16	1/2-X,	1/2+Y,	1/4-Z

17	X,	Y,	1/2+Z
18	-X,	-Y,	1/2+Z
19	-Y,	X,	3/4+Z
20	Y,	-X,	3/4+Z
21	Y,	X,	1/2-Z
22	-Y,	-X,	1/2-Z
23	X,	-Y,	3/4-Z
24	-X,	Y,	3/4-Z

25	1/2+X,	1/2+Y,	1/2+Z
26	1/2-X,	1/2-Y,	1/2+Z
27	1/2-Y,	1/2+X,	3/4+Z
28	1/2+Y,	1/2-X,	3/4+Z
29	1/2+Y,	1/2+X,	1/2-Z
30	1/2-Y,	1/2-X,	1/2-Z
31	1/2+X,	1/2-Y,	3/4-Z
32	1/2-X,	1/2+Y,	3/4-Z

Verify your answer x,y,z is consistent with space group $P4_32_12$.

- There is only a 50% probability that our heavy atom coordinates (x,y,z) are consistent with space group $P4_32_12$. The remaining 50% probability is that x,y,z is consistent with space group $P4_12_12$, even though we used $P4_32_12$ symmetry operators to derive our coordinates and our algebra is faultless.
- Space group $P4_32_12$ is chiral, meaning that it contains symmetry elements of a particular hand. For example, the 4_3 axis in $P4_32_12$ is a left handed screw.
- Space group $P4_12_12$ is also chiral, and its symmetry elements are the mirror image of space group $P4_32_12$.



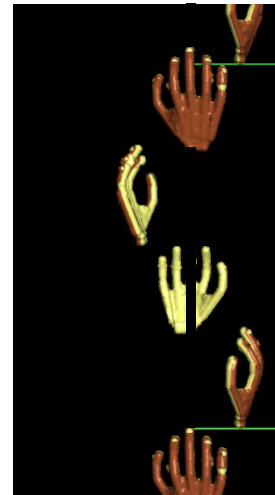
Right hand screw

Left hand screw

Verify your answer x,y,z is consistent with space group $P4_32_12$.

- Crystals in chiral space groups $P4_12_12$ and $P4_32_12$ share the same Patterson symmetry group, $P4/mmm$, which is not chiral, but centrosymmetric.
- All Patterson maps (including $P4/mmm$) are centrosymmetric because their peaks represent vectors between atoms. Every pair of atoms is connected by two vectors of equal length and opposite direction: $\text{atom1} \rightarrow \text{atom2}$ and $\text{atom1} \leftarrow \text{atom2}$, thereby creating centrosymmetry.
- The 50% chance of space group inconsistency arises from our unavoidable dependence on a centrosymmetric map to derive coordinates in a chiral space group.
- Among the 230 space groups, only 22 are chiral. How did we get so lucky to stumble one of these?

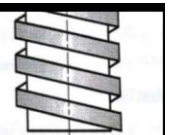
4_1



4_3



Right hand screw

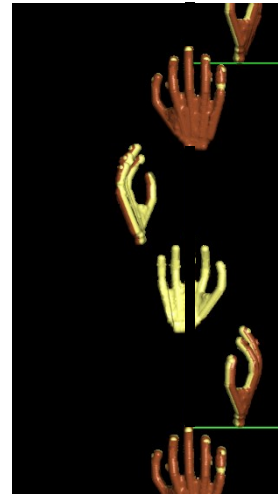


Left hand screw

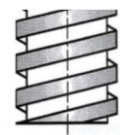
Verify your answer x,y,z is consistent with space group $P4_32_12$.

- The heavy atom coordinates (x,y,z) are verified to be consistent with space group $P4_32_12$ if (x,y,z) if it can be used to successfully predict coordinates (u,v,w) of a non-Harker Patterson peak.
- If prediction is unsuccessful, invert the hand of the heavy atom solution by negating x to make it compatible with $P4_32_12$.

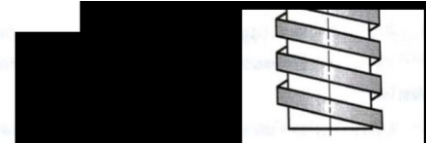
4_1



4_3

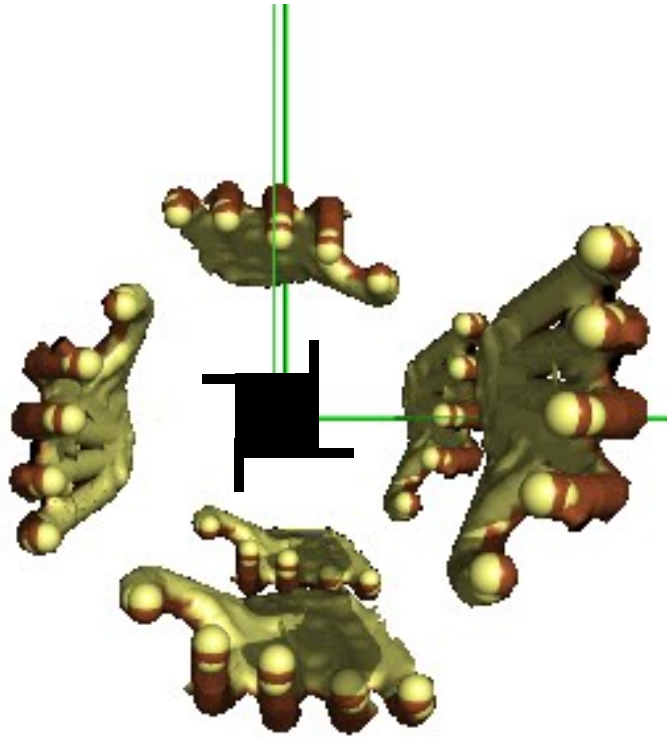


Right hand screw



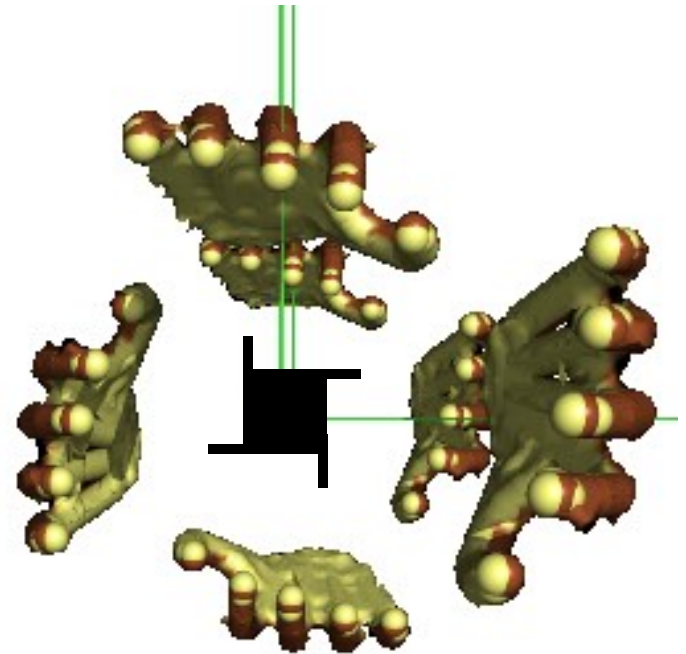
Left hand screw

Verify your answer x,y,z is consistent with space group $P4_32_12$.



4_1

Right hand screw



4_3

Left hand screw

1)	x	y	z
2)	-x	-y	1/2+z
	2x	2y	-1/2

Table of Patterson Difference Vectors (U,V,W)

1)	x	y	z
3)	1/2-y	1/2+x	3/4+z
	-1/2+x+y	-1/2-x+y	-3/4

2)	-x	-y	1/2+z
3)	1/2-y	1/2+x	3/4+z
	-1/2-x+y	-1/2-x-y	-1/4

1)	x	y	z
4)	1/2+y	1/2-x	1/4+z
	-1/2+x-y	-1/2+x+y	-1/4

2)	-x	-y	1/2+z
4)	1/2+y	1/2-x	1/4+z
	-1/2-x-y	-1/2+x-y	1/4

3)	1/2-y	1/2+x	3/4+z
4)	1/2+y	1/2-x	1/4+z
	-2y	2x	1/2

1)	x	y	z
5)	y	x	-z
	x-y	-x+y	2z

2)	-x	-y	1/2+z
5)	y	x	-z
	-x-y	-x-y	1/2+2z

3)	1/2-y	1/2+x	3/4+z
5)	y	x	-z
	1/2-2y	1/2	3/4+2z

4)	1/2+y	1/2-x	1/4+z
5)	y	x	-z
	1/2	1/2-2x	1/4+2z

1)	x	y	z
6)	-y	-x	1/2-z
	x+y	x+y	-1/2+2z

2)	-x	-y	1/2+z
6)	-y	-x	1/2-z
	-x+y	x-y	2z

3)	1/2-y	1/2+x	3/4+z
6)	-y	-x	1/2-z
	1/2	1/2+2x	1/4+2z

4)	1/2+y	1/2-x	1/4+z
6)	-y	-x	1/2-z
	1/2+2y	1/2	-1/4+2z

5)	y	x	-z
6)	-y	-x	1/2-z
	2y	2x	-1/2

1)	x	y	z
7)	1/2-x	1/2+y	3/4-z
	-1/2+2x	-1/2	-3/4+2z

2)	-x	-y	1/2+z
7)	1/2-x	1/2+y	3/4-z
	-1/2	-1/2-2y	-1/4+2z

3)	1/2-y	1/2+x	3/4+z
7)	1/2-x	1/2+y	3/4-z
	x-y	x-y	2z

4)	1/2+y	1/2-x	1/4+z
7)	1/2-x	1/2+y	3/4-z
	x+y	-x-y	-1/2+2z

5)	y	x	-z
7)	1/2-x	1/2+y	3/4-z
	-1/2+x+y	-1/2+x-y	-3/4

6)	-y	-x	1/2-z
7)	1/2-x	1/2+y	3/4-z
	-1/2-x-y	-1/2-x-y	-1/4

1)	x	y	z
8)	1/2+x	1/2-y	1/4-z
	-1/2	-1/2+2y	-1/4+2z

2)	-x	-y	1/2+z
8)	1/2+x	1/2-y	1/4-z
	-1/2-2x	-1/2	1/4+2z

3)	1/2-y	1/2+x	3/4+z
8)	1/2+x	1/2-y	1/4-z
	-x-y	x+y	1/2+2z

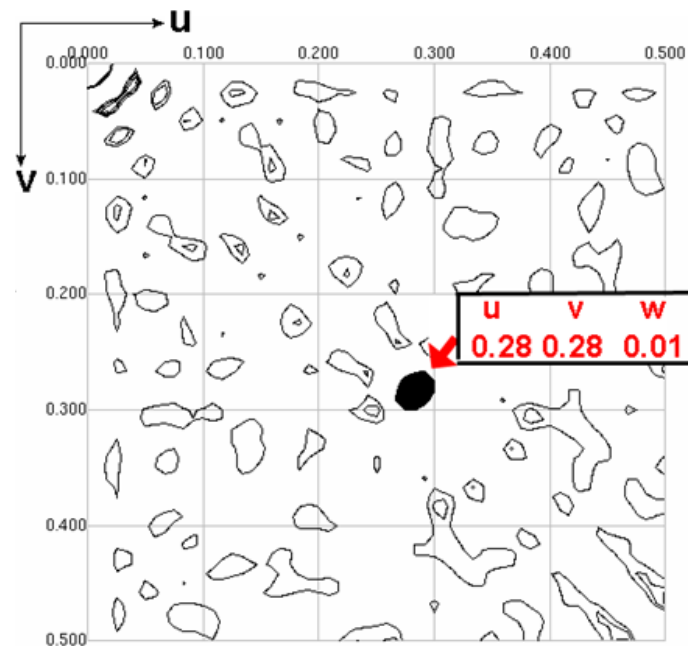
4)	1/2+y	1/2-x	1/4+z
8)	1/2+x	1/2-y	1/4-z
	-x+y	-x+y	2z

5)	y	x	-z
8)	1/2+x	1/2-y	1/4-z
	-1/2-x+y	-1/2+x+y	-1/4

6)	-y	-x	1/2-z
8)	1/2+x	1/2-y	1/4-z
	-1/2-x-y	-1/2-x+y	1/4

7)	1/2-x	1/2+y	3/4-z
8)	1/2+x	1/2-y	1/4-z
	-2x	2y	1/2

isomorphous difference Patterson map
w= 0.01



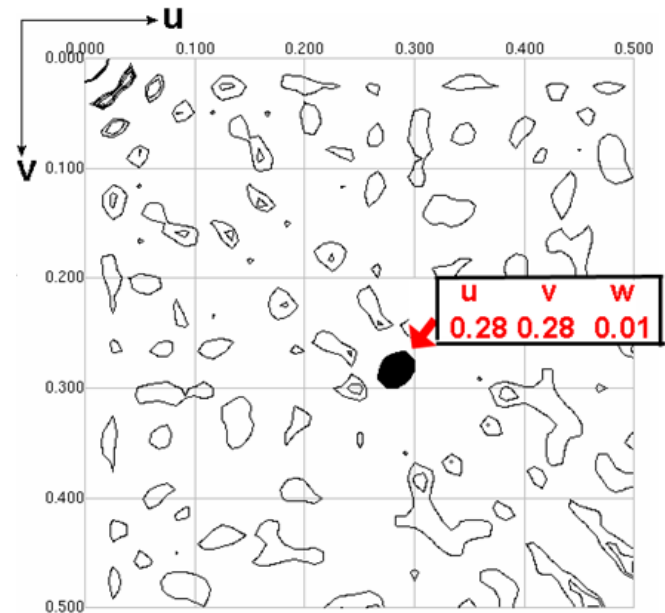
Plug in x,y,z and solve for u,v,w of a non-Harker Patterson peak

Original x,y,z

$$x=-0.020, y=+0.700, z=-0.005$$

symop 1	x	y	z
-symop 5	-(y	x	-z)
	u=x-y	v=-x+y	w=2z

isomorphous difference Patterson map
w= 0.01



Plug in x,y,z and solve for u,v,w of a non-Harker Patterson peak

Original x,y,z

$$x = -0.020, y = +0.700, z = -0.005$$

$$\begin{array}{rcll} \text{symop } 1 & x & y & z \\ \hline \text{-symop } 5 & -(y & x & -z) \\ & u=x-y & v=-x+y & w=2z \end{array}$$

$$u = x - y$$

$$u = -0.020 - 0.700$$

$$u = -0.720$$

$$v = -x + y$$

$$v = +0.020 + 0.700$$

$$v = +0.720$$

$$w = 2z$$

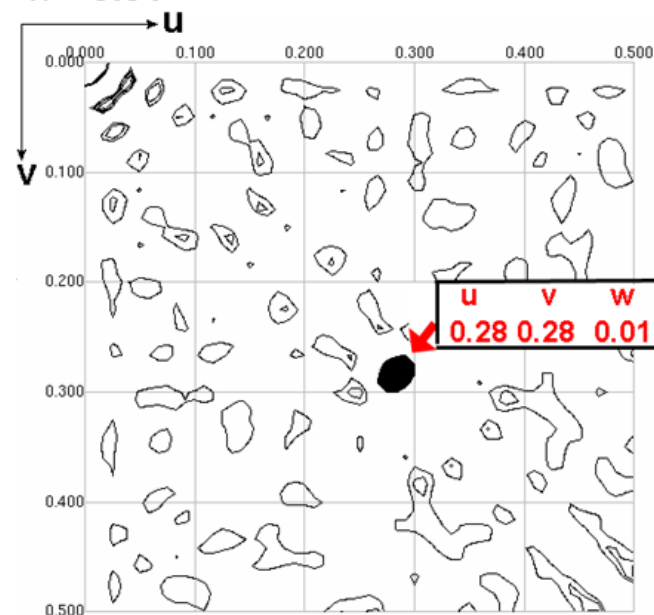
$$w = 2(-0.005)$$

$$w = -0.010$$

Note: u,v,w values lay outside the section drawn.

$$u = -0.72, v = 0.72, w = -0.01$$

isomorphous difference Patterson map
w = 0.01



Plug in x,y,z and solve for u,v,w of a non-Harker Patterson peak

Original x,y,z

$$x = -0.020, y = +0.700, z = -0.005$$

$$\begin{array}{rcll} \text{symop } 1 & x & y & z \\ \hline \text{-symop } 5 & -(y & x & -z) \\ & u=x-y & v=-x+y & w=2z \end{array}$$

$$\begin{aligned} u &= x - y \\ u &= -0.020 - 0.700 \\ u &= -0.720 \end{aligned}$$

$$\begin{aligned} v &= -x + y \\ v &= +0.020 + 0.700 \\ v &= +0.720 \end{aligned}$$

$$\begin{aligned} w &= 2z \\ w &= 2(-0.005) \\ w &= -0.010 \end{aligned}$$

Note: u,v,w values lay outside the section drawn.

$$u = -0.72, v = 0.72, w = -0.01$$

Apply Patterson symmetry to transform coordinates to values between 0.0 and 0.5.

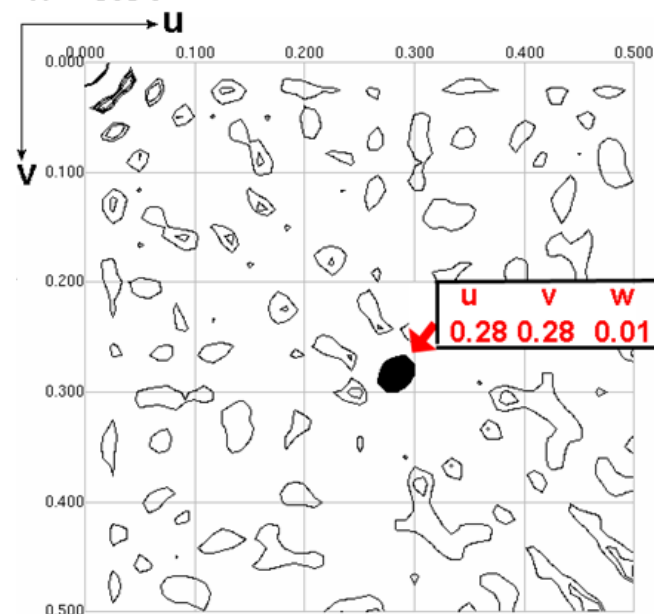
- | | | | |
|--------------|----------------|----------------|-----------------|
| (1) U, V, W | (2) -U, -V, W | (3) U, V, -W | (4) -U, -V, -W |
| (5) -U, V, W | (6) U, -V, W | (7) -U, V, -W | (8) U, -V, -W |
| (9) -V, U, W | (10) V, -U, W | (11) -V, U, -W | (12) V, -U, -W |
| (13) V, U, W | (14) -V, -U, W | (15) V, U, -W | (16) -V, -U, -W |

Apply operation 1+u,1-v,-w

$u = 0.28, v = 0.28, w = 0.01$ which matches the peak shown here.

Thus, $x = -0.02, y = 0.70, z = -0.005$ is correct.
Hurray! We are finished!

isomorphous difference Patterson map
 $w = 0.01$



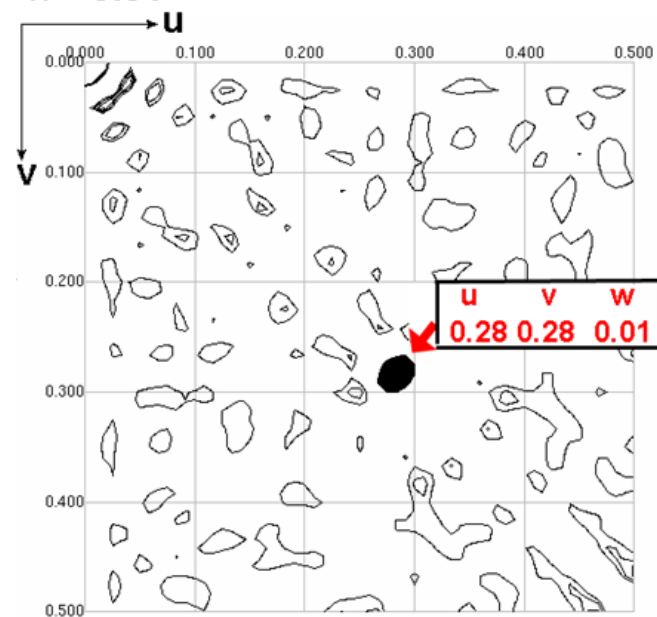
An example when the x,y,z does **not** predict u,v,w .

Original x,y,z

$x=+0.020, y=+0.700, z=-0.005$

symop 1	x	y	z
-symop 5	$-(y$	x	$-z)$
	$u=x-y$	$v=-x+y$	$w=2z$

isomorphous difference Patterson map
 $w=0.01$



An example when the x,y,z does **not** predict u,v,w .

Original x,y,z

$x=+0.020, y=+0.700, z=-0.005$

symop 1	x	y	z
-symop 5	$-(y$	x	$-z)$
	$u=x-y$	$v=-x+y$	$w=2z$

$u=x-y$
$u= 0.020-0.700$
$u=-0.680$

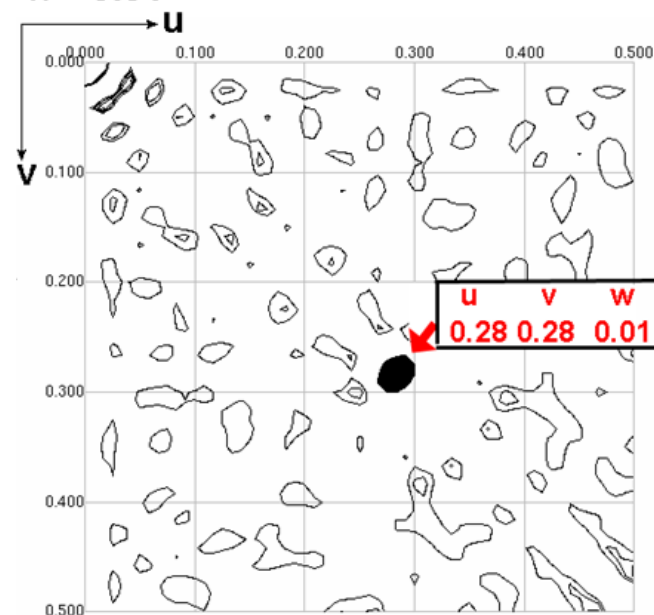
$v=-x+y$
$v=-0.020+0.700$
$v= 0.680$

$w=2z$
$w=2(-0.005)$
$w=-0.010$

Note: u,v,w values lay outside the section drawn.

$u= -0.68, v= 0.68, w= -0.01$

isomorphous difference Patterson map
 $w= 0.01$



An example when the x,y,z does **not** predict u,v,w.

Original x,y,z

$$x=+0.020, y=+0.700, z=-0.005$$

$$\begin{array}{rcl} \text{symop } 1 & x & y & z \\ \hline \text{-symop } 5 & -(y & x & -z) \\ & u=x-y & v=-x+y & w=2z \end{array}$$

$$u=x-y$$

$$u=0.020-0.700$$

$$u=-0.680$$

$$v=-x+y$$

$$v=-0.020+0.700$$

$$v=0.680$$

$$w=2z$$

$$w=2(-0.005)$$

$$w=-0.010$$

Note: u,v,w values lay outside the section drawn.

$$u=-0.68, v=0.68, w=-0.01$$

Apply Patterson symmetry to transform coordinates to values between 0.0 and 0.5.

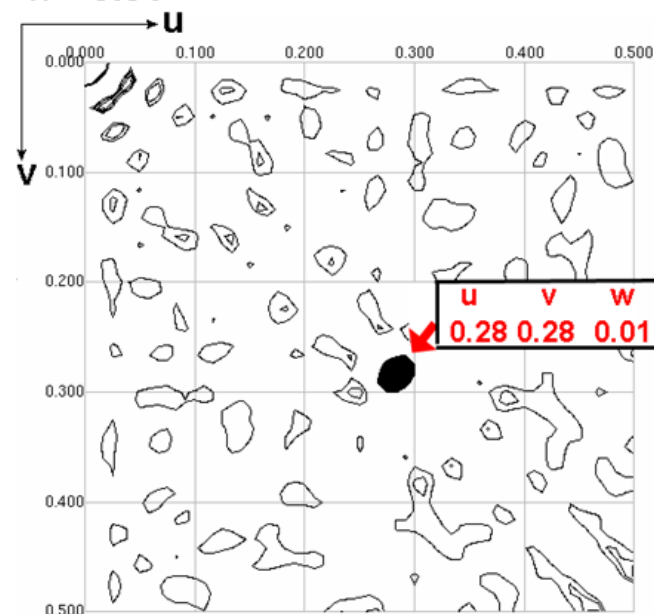
- | | | | |
|--------------|----------------|----------------|-----------------|
| (1) U, V, W | (2) -U, -V, W | (3) U, V, -W | (4) -U, -V, -W |
| (5) -U, V, W | (6) U, -V, W | (7) -U, V, -W | (8) U, -V, -W |
| (9) -V, U, W | (10) V, -U, W | (11) -V, U, -W | (12) V, -U, -W |
| (13) V, U, W | (14) -V, -U, W | (15) V, U, -W | (16) -V, -U, -W |

Apply operation 1+u,1-v,-w

$u=0.32, v=0.32, w=0.01$ which does **not** match the peak shown here.

In this case we would negate x and recalculate u,v,w again. Then you should find the match.

isomorphous difference Patterson map
 $w=0.01$



In Lab next week

- We have several native data sets and several Hg, Eu, and Gd derivative data sets.
- Each person will calculate a difference Patterson map involving the data they collected.
 - Anomalous difference Patterson map
 - Isomorphous difference Patterson map
- We will record the height of the highest peak on the $w=0.5$ section for each map.
- The native-derivative pair with the highest peak will be used by the whole class.
- We will all interpret the difference Patterson map to calculate coordinates x,y,z for the heavy atom.
- Perform the calculations carefully. Incorrect x,y,z will produce an uninterpretable electron density map.
- Bring your correct choice of x,y,z to Phasing lab the following week and we will calculate and view an electron density map.

Caution

- Algebra is simple.
- You will feel compelled to abbreviate your algebraic steps in order to finish early.
- Abbreviating algebra is the kiss of death.
- Write each step, don't combine steps.
- Write neatly.
- Keep track of negative signs.
- Use worksheets.

END OF PRESENTATION

Advanced case, Proteinase K in space group $P4_32_12$

- How many Patterson peaks?
- Where are Harker sections?

$P4_32_12$

No. 96

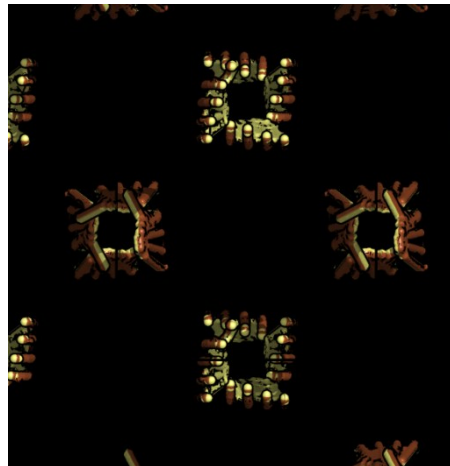
D_4^8

$P4_32_12$

422

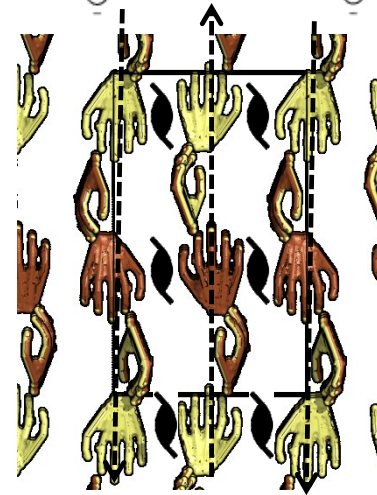
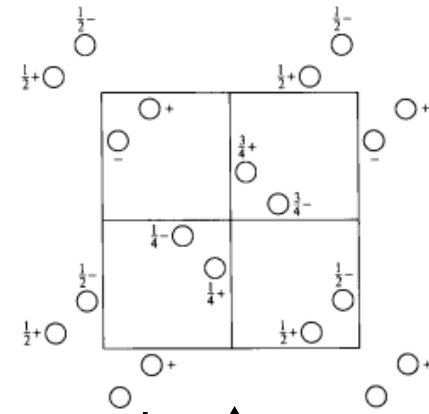
Tetragonal

Patterson symmetry $P4/mmm$



Origin on $2[110]$ at $2_11(1,2)$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}$



1 x, y, z

2 $\bar{x}, \bar{y}, \frac{1}{2} + z$

3 $\frac{1}{2} - y, \frac{1}{2} + x, \frac{3}{4} + z$

4 $\frac{1}{2} + y, \frac{1}{2} - x, \frac{1}{4} + z$

5 $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{4} - z$

6 $\frac{1}{2} - x, \frac{1}{2} + y, \frac{3}{4} - z$

7 $\bar{y}, \bar{x}, \frac{1}{2} - z$

8 $y, x, \bar{z}$

Advanced case, Proteinase K in space group $P4_32_12$

- How many Patterson peaks?
- Where are Harker sections?

1 x, y, z

2 $\bar{x}, \bar{y}, \frac{1}{2} + z$

3 $\frac{1}{2} - y, \frac{1}{2} + x, \frac{3}{4} + z$

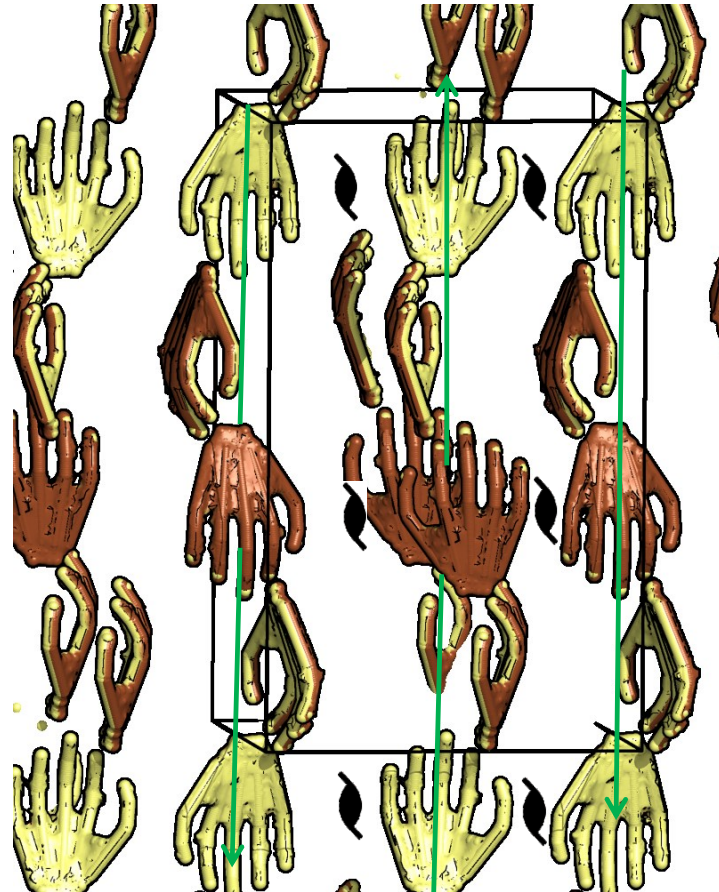
4 $\frac{1}{2} + y, \frac{1}{2} - x, \frac{1}{4} + z$

5 $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{4} - z$

6 $\frac{1}{2} - x, \frac{1}{2} + y, \frac{3}{4} - z$

7 $\bar{y}, \bar{x}, \frac{1}{2} - z$

8 $y, x, \bar{z}$



Advanced case, Proteinase K in space group $P4_32_12$

- How many Patterson peaks?
- Where are Harker sections?

1 x, y, z reference

2 $\bar{x}, \bar{y}, \frac{1}{2} + z$ 180° around z, translate $\frac{1}{2}$ along z

3 $\frac{1}{2} - y, \frac{1}{2} + x, \frac{3}{4} + z$ 270° around z, translate $\frac{3}{4}$ along z

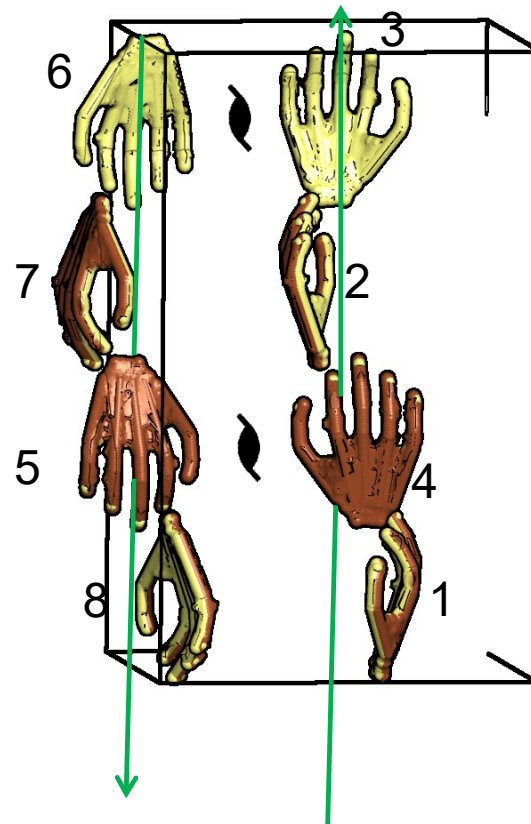
4 $\frac{1}{2} + y, \frac{1}{2} - x, \frac{1}{4} + z$ 90° around z, translate $\frac{1}{4}$ along z

5 $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{4} - z$

6 $\frac{1}{2} - x, \frac{1}{2} + y, \frac{3}{4} - z$

7 $\bar{y}, \bar{x}, \frac{1}{2} - z$

8 $y, x, \bar{z}$



$$\begin{array}{rcl}
 \text{sym operator 1} & \mathbf{x} & \mathbf{y} & \mathbf{z} \\
 \hline
 \text{-sym operator 5} & -(\mathbf{y} & \mathbf{x} & -\mathbf{z}) \\
 \hline
 \mathbf{u=x-y} & \mathbf{v=-x+y} & \mathbf{w=2z}
 \end{array}$$

Original x

$$\mathbf{x=-0.020, y=+0.700, z=-0.005}$$

Negated x

$$\mathbf{x=+0.020, y=+0.700, z=-0.005}$$

$\mathbf{u=x-y}$	$\mathbf{v=-x+y}$	$\mathbf{w=2z}$
$\mathbf{u=-0.020-0.700}$	$\mathbf{v=+0.020+0.700}$	$\mathbf{w=2(-0.005)}$
$\mathbf{u=-0.720}$	$\mathbf{v=+0.720}$	$\mathbf{w=-0.010}$

$\mathbf{u=x-y}$	$\mathbf{v=-x+y}$	$\mathbf{w=2z}$
$\mathbf{u=+0.020-0.700}$	$\mathbf{v=-0.020+0.700}$	$\mathbf{w=2(-0.005)}$
$\mathbf{u=-0.680}$	$\mathbf{v=+0.680}$	$\mathbf{w=-0.010}$

Note: u,v,w values lay outside the section drawn.
 $\mathbf{u=-0.72, v=0.72, w=-0.01}$

Apply Patterson symmetry to transform coordinates to values between 0.0 and 0.5.

(1) U, V, W	(2) -U, -V, W	(3) U, V, -W	(4) -U, -V, -W
(5) -U, V, W	(6) U, -V, W	(7) -U, V, -W	(8) U, -V, -W
(9) -V, U, W	(10) V, -U, W	(11) -V, U, -W	(12) V, -U, -W
(13) V, U, W	(14) -V, -U, W	(15) V, U, -W	(16) -V, -U, -W

Apply operation 1+u,1-v,-w

$\mathbf{u=0.28, v=0.28, w=0.01}$ which matches the peak coordinates.

Thus, $\mathbf{x=-0.020, y=0.700, z=-0.005}$ is correct.
 Hurray! We are finished!

Note: u,v,w values lay outside the section drawn.
 $\mathbf{u=+0.68, v=-0.68, w=-0.01}$

Apply Patterson symmetry to transform coordinates to values between 0.0 and 0.5.

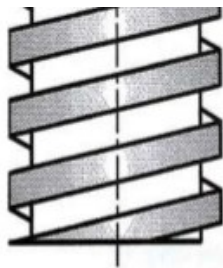
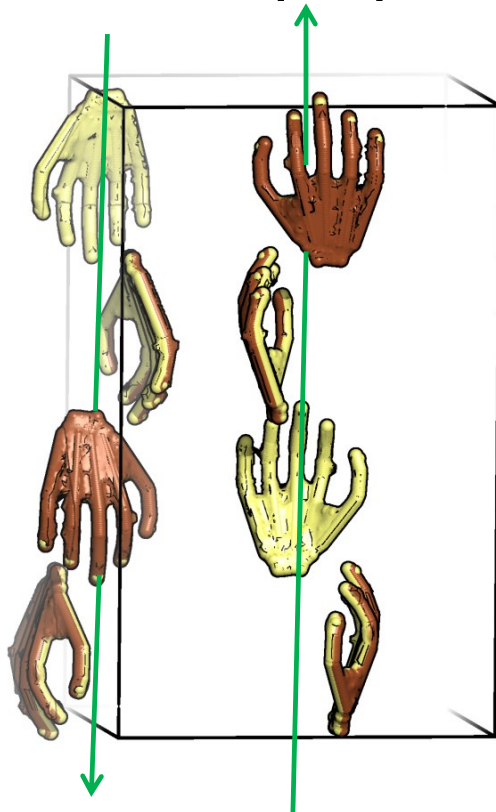
(1) U, V, W	(2) -U, -V, W	(3) U, V, -W	(4) -U, -V, -W
(5) -U, V, W	(6) U, -V, W	(7) -U, V, -W	(8) U, -V, -W
(9) -V, U, W	(10) V, -U, W	(11) -V, U, -W	(12) V, -U, -W
(13) V, U, W	(14) -V, -U, W	(15) V, U, -W	(16) -V, -U, -W

Apply operation 1-u,1+v,-w

$\mathbf{u=0.32, v=0.32, w=0.01}$ which does NOT match non-Harker peak.

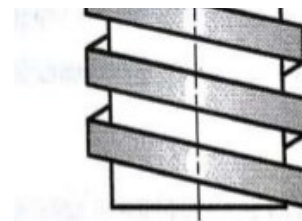
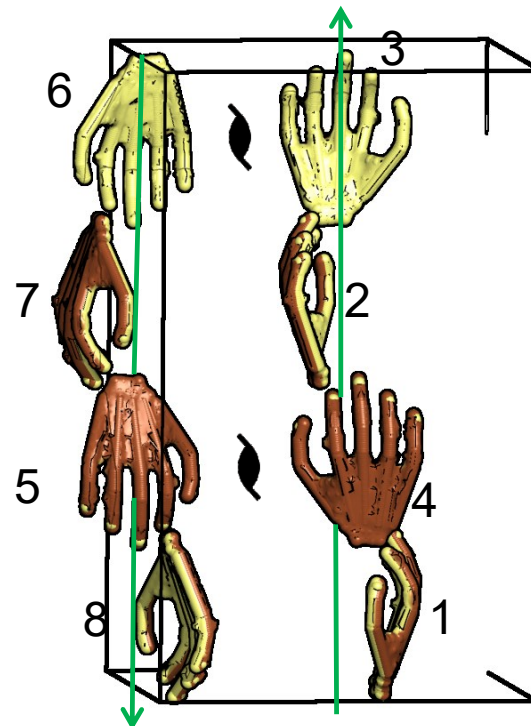
Original x was correct.

$P4_12_12$



(a) Right Hand Threads

$P4_32_12$



(b) Left Hand Threads

m230d_2015_scaled2.mtz

All data sets were entered in a spreadsheet.

Each column label a different measured quantity. Each row specifies a different HKL.

-using the CCP4 program CAD.

	H	K	L	FreeR_flag	FP_native-jeannette	SIGFP_native-jeannette	FP_native-john	SIGFP_native-john	FP_native-aj	SIGFP_native-aj	FP_native-joshua	SIGFP_native-joshua	FP_native-mimi	SIGFP_native-mimi	FP_native-wenyang	SIGFP_native-wenyang	FP_eucl3-beccah	SIGFP_eucl3-beccah	D_eucl3-beccah	SIGD_eucl3-beccah	FP_eucl3-jessica	SIGFP_eucl3-jessica	D_eucl3-jessica	SIGD_eucl3-jessica	Up to 72 columns
3 2 64			10.00	130.30	2.20	174.93	2.12	150.51	4.01	144.96	2.04	103.41	4.04	164.00	2.62	126.54	1.31	6.82	2.62	149.88	1.83	-0.66	3.67		
3 2 65			9.00	175.48	1.66	191.37	2.00	197.89	3.23	177.46	1.75	159.61	2.69	202.44	2.22	180.36	1.13	5.15	2.26	170.56	1.66	-0.73	3.31		
3 2 66			17.00	110.19	2.60	129.09	2.69	141.68	4.54	121.00	2.29	82.97	5.16	165.87	2.24	97.76	1.65	4.36	3.30	103.57	2.45	-5.45	4.89		

Etc. for thousands of reflections

Scale intensities by a constant (k) and resolution dependent exponential (B)

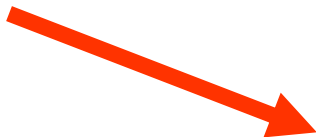
prok-native-yen

H	K	L	intensity	sigma
1	0	10	106894.0	1698.0
1	0	11	41331.5	702.3
1	0	12	76203.2	1339.0
1	0	13	28113.5	513.6
1	0	14	6418.2	238.7
1	0	15	45946.4	882.7
1	0	16	26543.8	555.6

prok-gdcl3-matthew

H	K	L	intensity	sigma
1	0	10	40258.7	1222.9
1	0	11	25033.2	799.8
1	0	12	24803.6	771.5
1	0	13	11486.3	423.9
1	0	14	9180.5	353.6
1	0	15	25038.8	783.0
1	0	16	21334.6	686.4

comparison


$$\begin{aligned}106894.0 &/ 40258.7 = 2.65 \\41331.5 &/ 25033.2 = 1.65 \\76203.2 &/ 24803.6 = 3.07 \\28113.5 &/ 11486.3 = 2.45 \\6418.2 &/ 9180.5 = 0.70 \\45946.4 &/ 25038.8 = 1.83 \\26543.8 &/ 21334.6 = 1.24\end{aligned}$$

-Probably **first** crystal is larger than the **second**.

-Multiply Saken's data by k and B to put the data on the same scale.

m230d_2015_scaled2.mtz

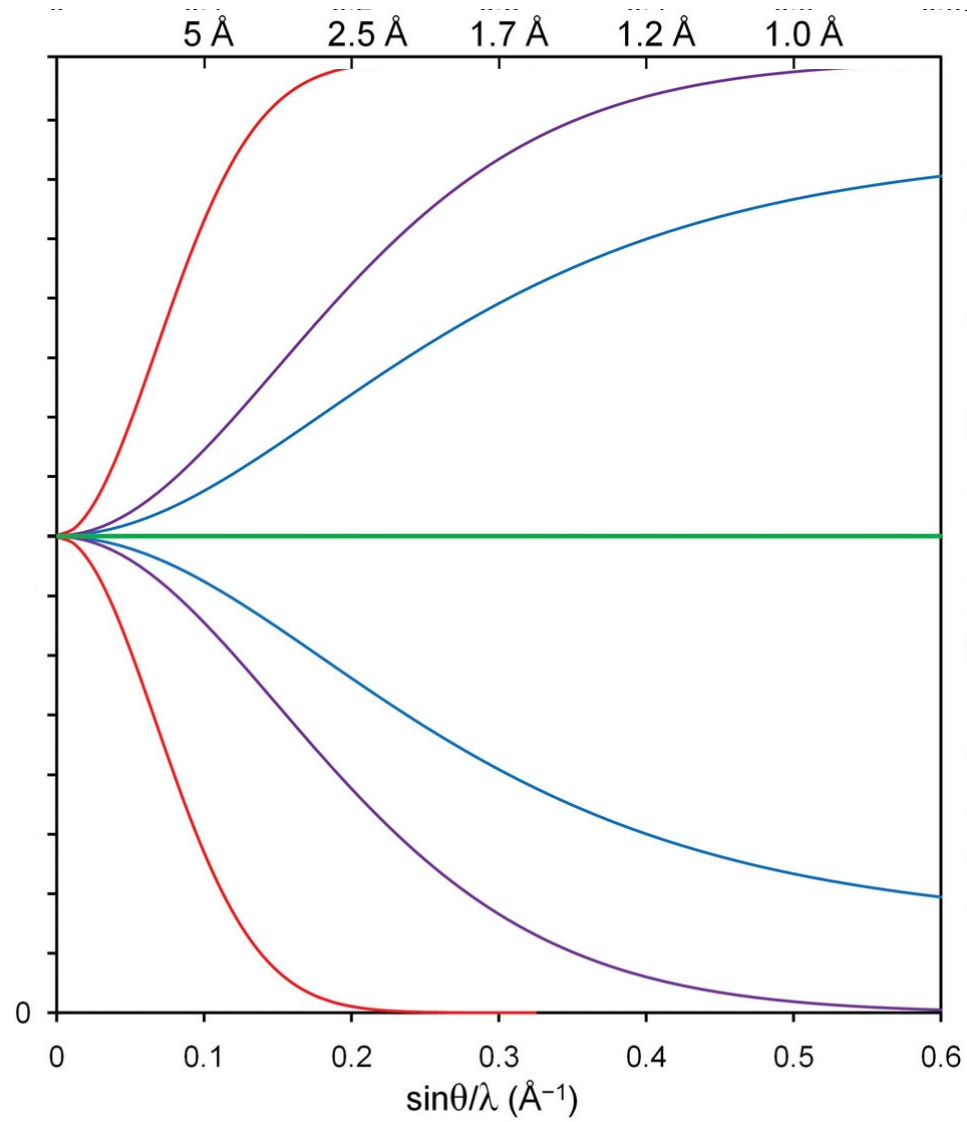
Intensity measurements were converted to structure factor amplitudes ($|F_{\text{HKL}}|$)

-using the CCP4 program TRUNCATE.

All data sets were scaled to a reference native data set with the best statistics: prok-native-jeannette

-using the CCP4 program SCALEIT.

$$e^{-B^* \sin^2 \theta / \lambda^2}$$



- Dear Sung Chul,
- I apologize for the lack of clarity. Both x,y,z and $-x,y,z$ can satisfy the vector equations in step 6 because both the Harker sections used thus far contain mirror symmetry that is consistent with either sign of "x". In other words, the peaks in these Harker sections are related by Patterson symmetry that makes them consistent with either sign of "x"
- However, there are other difference vector equations in this space group (for example symop 1 - symop 5) that are not reflected by these mirror planes. These can be used to discriminate which sign of "x" is correct. Only one of these choices of the sign of "x" will be able to predict correctly Patterson peaks specified by this difference vector.
- My thought is that one sign of "x" is consistent with space group P43212, and the other sign of "x" is consistent with space group P41212.
- Mike
- On 01/08/2015 06:21 PM, 하성철 wrote:
 - >
 - > Dear Michael R. Sawaya,
 - >
 - >
 - >
 - > I have learned a lot basic concept and practical methods using presentation materials of the lectures for CHEM M230D Course. They are prepared well so that anyone can understand the contents easily even without the explanation by a lecturer.
 - >
 - >
 - >
 - > I have one question about content of the presentation ppt file for the lectures for CHEM M230D Course. In the ppt file or on the web page for "Difference Patterson Maps and Determination of Heavy Atom Sites", I don't know why both x,y,z and $-x,y,z$ can satisfy the difference vector equations in the step 6. Could you explain the reason?
 - >
 - >
 - >
 - > Best regards,
 - >
 - > SungChul Ha
 - >
 - >

Patterson Review

A Patterson synthesis is like a Fourier synthesis except for what two variables?

Fourier synthesis

$$\rho_{x y z} = \sum_{hkl} |F_{hkl}| \cos 2\pi(hx + ky + lz - \alpha_{hkl})$$

Patterson synthesis

$$P_{u v w} = \sum_{hkl} I_{hkl} \cos 2\pi(hu + kv + lw - 0)$$

Peak coordinates (u,v,w) indicate vectors between atoms in the unit cell.

$$P_{u\ v\ w} = \rho_{x\ y\ z} \otimes \rho_{-x\ -y\ -z}$$

Patterson map= electron density map convoluted with its inverted image.

- Conceptual image of a Patterson map.
 - Suppose you knew the coordinates of all atoms in a unit cell.
 - Imagine a vector connecting every pair of atoms.
 - Translate each vector so tail is at the origin.
 - Peak is located at the head of the vector.
 - That's a Patterson map.
 - If n atoms in unit cell, then n^2 peaks in Patterson.
 - Both forward and reverse vectors included (centrosymmetric).
 - Includes vector between each atom and itself (0 length).
- If 2000 atoms in proteinase K derivative, 4 million Patterson peaks would result. Impossible to interpret.

Difference Patterson maps are simple enough to enable structure determination of a few heavy atoms.

Difference Patterson synthesis

$$P(uvw) = \sum_{hkl} |F_{PH(hkl)} - F_P(hkl)|^2 \cos 2\pi(hu + kv + lw - 0)$$

Heavy atom derivative amplitudes Native amplitudes

1. Vectors between protein atoms are subtracted away (remove 4 million peaks).
2. All remaining peaks correspond to vectors between heavy atoms only.
3. The reduced number of peaks makes it tractable to interpret the heavy atom coordinates x, y, z that produced peaks u, v, w .

Symmetry operators are listed in the Int'l Tables of Crystallography Vol A.

- Symmetry operators
 - (1) x, y, z
 - (2) $-x, -y, z$
 - (3) $-x + 1/2, y + 1/2, -z$
 - (4) $x + 1/2, -y + 1/2, -z$
 - Contains 2 and 2_1 axes perpendicular to each other.

Illustrate with
asymmetric unit=
Right hand



$P2_12_12_1$

No. 18

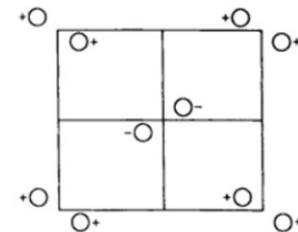
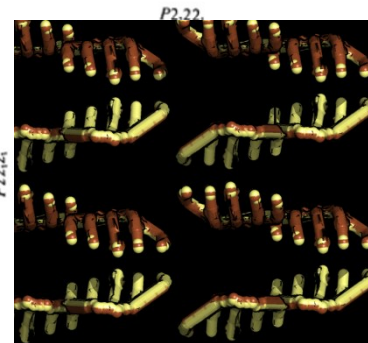
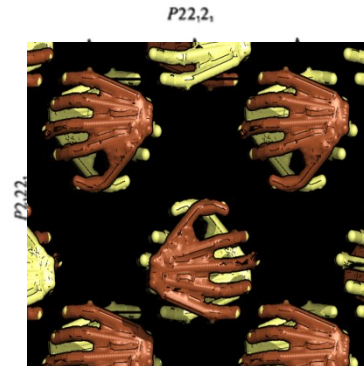
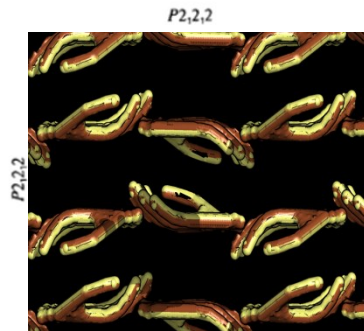
D_2^3

$P2_12_12_1$

222

Orthorhombic

Patterson symmetry $Pmmm$



Origin at intersection of 2 with perpendicular plane containing 2_1 axes

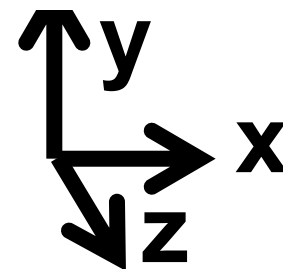
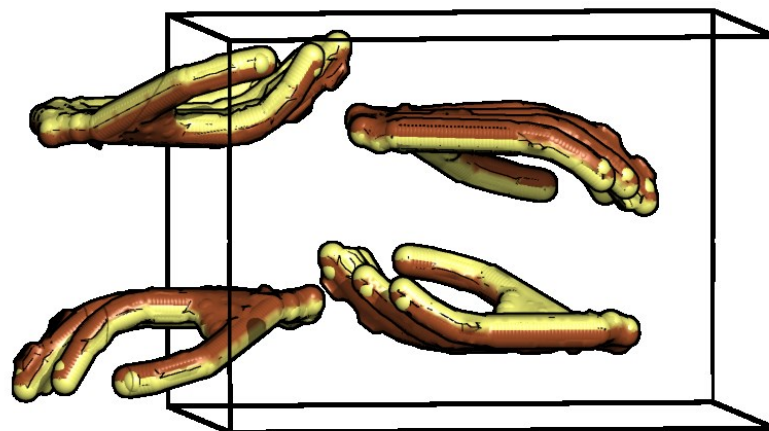
Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

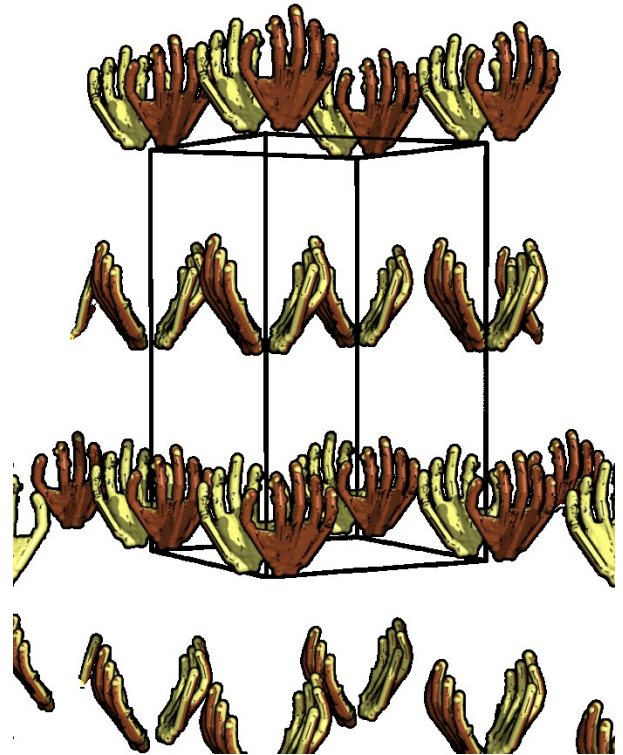
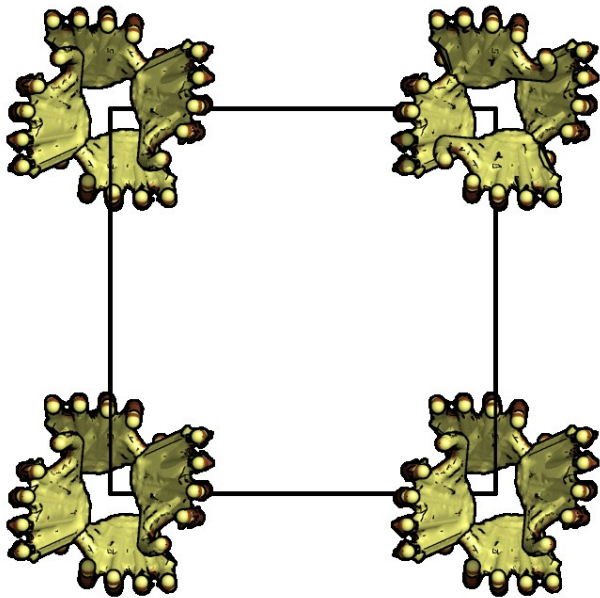
Pt derivative DNA polymerase β

$P2_12_12$

- (1) x, y, z
- (2) $-x, -y, z$
- (3) $-x + 1/2, y + 1/2, -z$
- (4) $x + 1/2, -y + 1/2, -z$

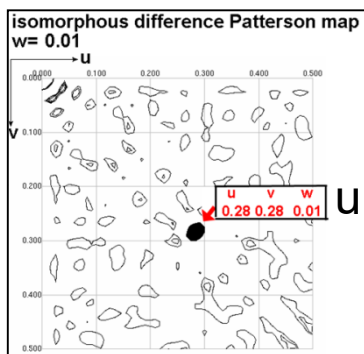
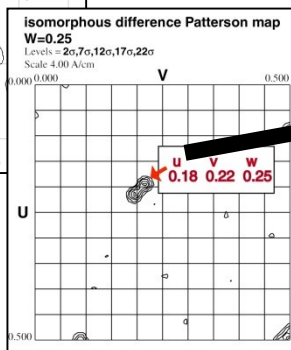
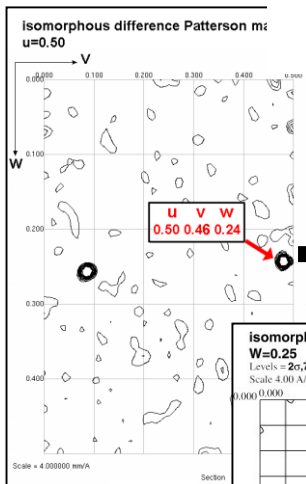


$P4_2$



Patterson space

Crystal space



U=0.5

P43212 Symmetry operator difference 3-6

W=0.25

P43212 Symmetry operator difference 2-4

Calculate Y and Z

Calculate X and Y

Cheshire operator applied to Y and Z if two values of Y do not match

X,Y,Z referred to a common origin.

Check answer for peak off Harker section.

P43212 Symmetry operator difference 1-5

$$\begin{array}{r} x \quad y \quad z \\ -(x \quad y \quad x \quad -z) \\ \hline x-y \quad -x+y \quad 2z \end{array}$$

u, v, w

If prediction lies outside Patterson asymmetric unit (0→0.5, 0→0.5, 0→0.5) use **Patterson symmetry operators** to find the symmetry equivalent peak in the asymmetric unit. If the predicted peak is absent, then negate x value and re-calculate u,v,w. Predicted peak should be present if algebra is correct.

Clues to Solving a Mystery:

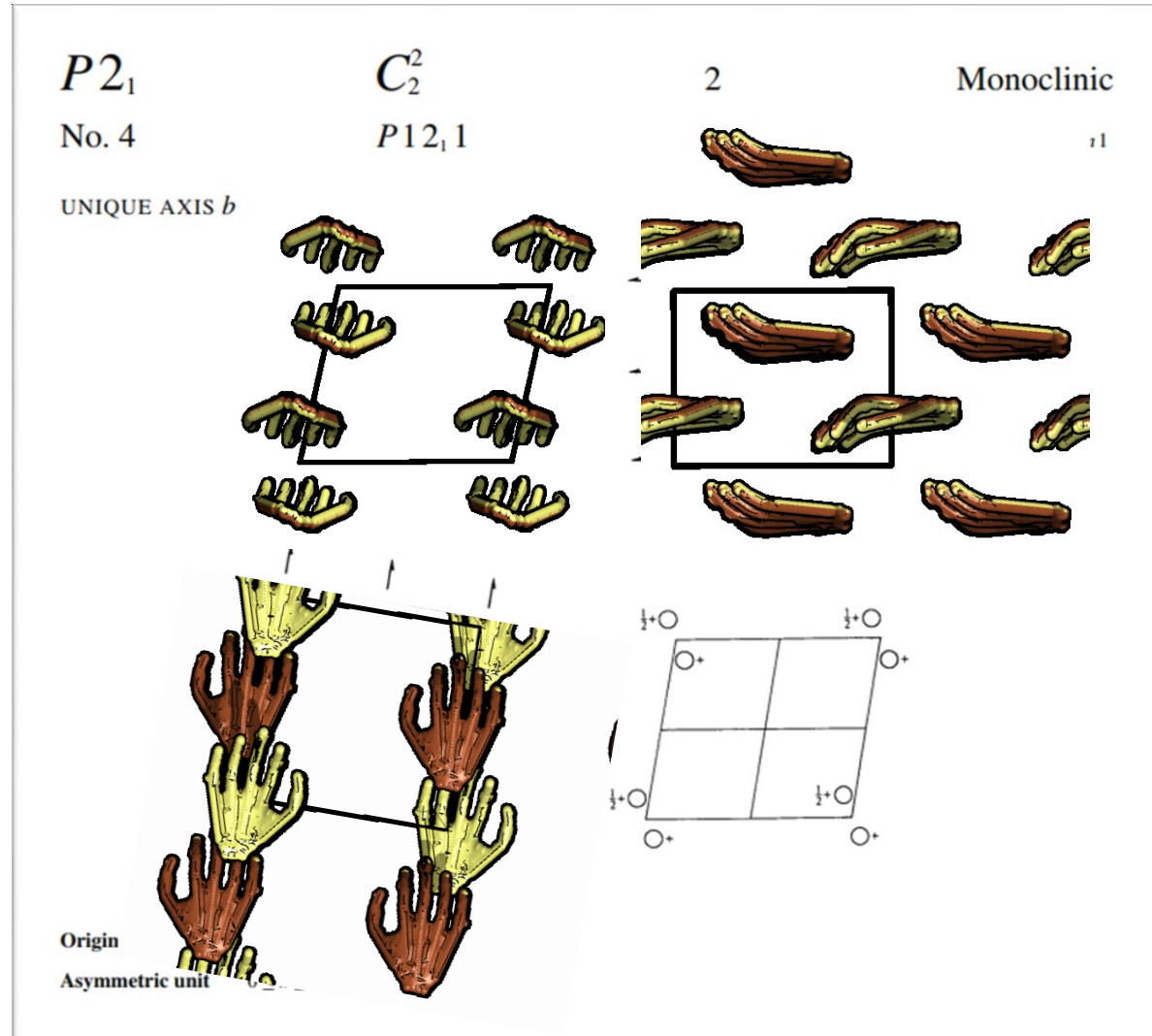
Locating Heavy Atom Coordinates x,y,z

- Each pair of heavy atoms is related by a vector, u,v,w . (read as coordinates of difference Patterson peak).
 - Gives distances between atoms and directions (a vector).
 - You can get coordinates of the heavy atoms relative to each other, but we want absolute coordinates, relative to origin, $(x,y,z)=0,0,0$
- To determine the heavy atom coordinates (x,y,z) relative to the origin (of the space group), realize that each difference Patterson peak (u,v,w) describes a vector between symmetry equivalent positions in the space group.
 - The vector is a difference between symmetry operators.
 - Symmetry operators are defined by the space group.
 - Must know the space group.
 - Must correctly assign Patterson peak to its pair of symmetry operators (or else you get wrong x,y,z).
- Harker sections reduce the ambiguity in assigning a peak to its symop pairs.
 - Take each pairwise difference between symmetry operators to locate all Harker sections in a space group.
 - Assign peaks on Harker sections to the corresponding symmetry operators.
- Solve for coordinates, (x,z) from 1st Harker section. Solve for (x,y) from 2nd Harker section. Never get all three coordinates from a single difference Patterson peak.
- Merge coordinates $(x,z)_{1st}$ with $(x,y)_{2nd}$ make a complete triplet, x,y,z .
 - Be careful that coordinates refer to same atom/origin (Cheshire operators)
- Check answer by predicting u,v,w from x,y,z .

Symmetry operators are listed in the Int'l Tables of Crystallography Vol A.

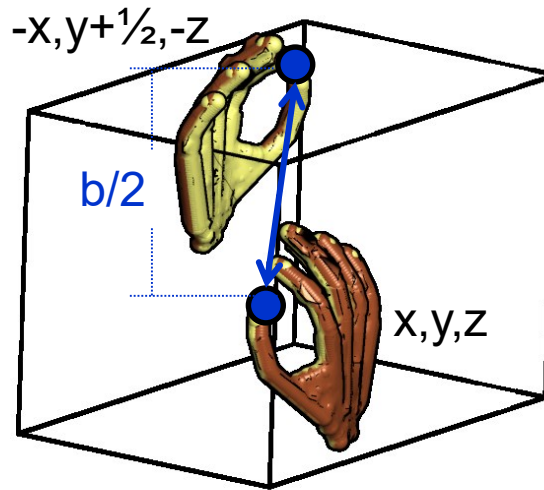
- Symmetry operators
 $Op1 = x, y, z$
 $Op2 = -x, y + \frac{1}{2}, -z$
- Space group conventions
- Projections of unit cell and symmetry.

Illustrate with
asymmetric unit=
Right hand

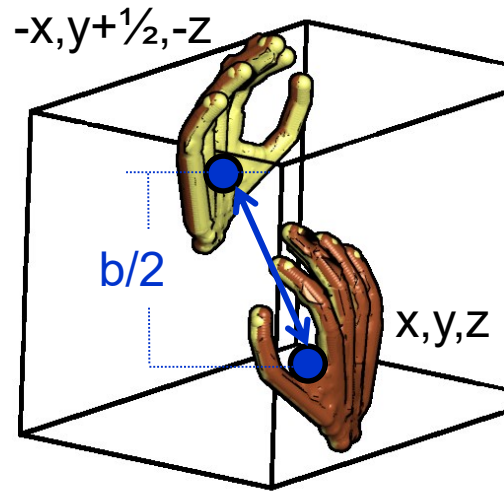


Note, in $P2_1$, the vector between heavy atoms always has v component = $\frac{1}{2}$.

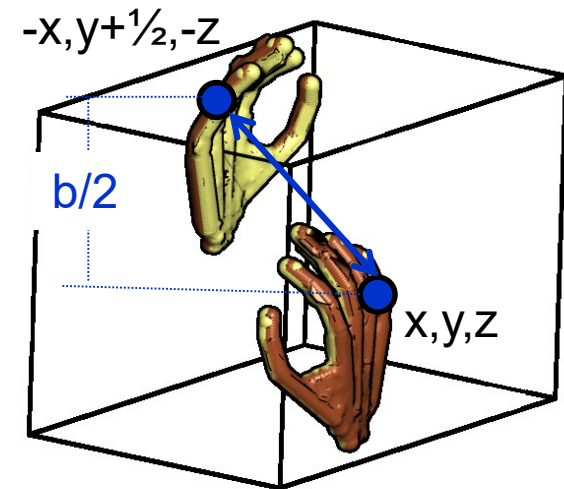
Pinched between thumb & forefinger



In the palm.



On the ring finger.

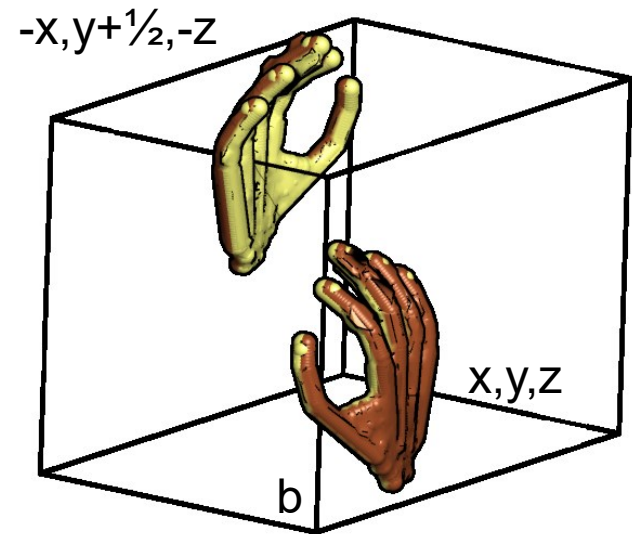


$P2_1$ is confined to be in the section $v = \frac{1}{2}$. Why?

- This plane $v = \frac{1}{2}$ is called a Harker section.

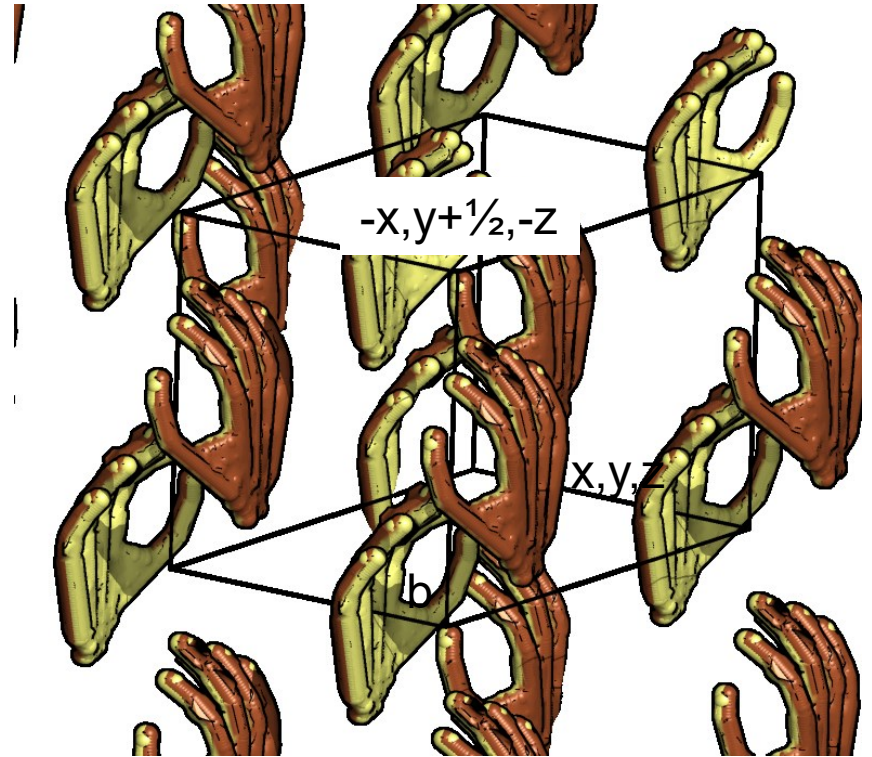
$P2_1$ symmetry in perspective

- Screw axis is along b .
- Two hands per unit cell.
- Symmetry operators specify how hands are related.
- For every feature at x, y, z , there is an equivalent feature at $-x, y + \frac{1}{2}, -z$



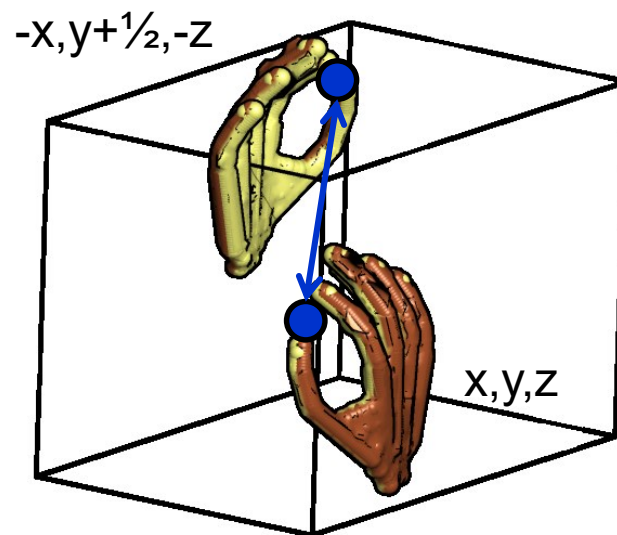
P2₁ symmetry in perspective

- All right hands
 - no mirrors or glide to produce left hands.



Write an expression for the Patterson peak coordinates of a heavy atom in $P2_1$

- Let's suppose a hand represents a molecule of NNQQNY.
- Let's suppose the Zn ion is pinched between the thumb and forefinger.
- What would the coordinates be for the expected Patterson peak?
- Take vector difference between symbolic coordinates. I call this a difference vector equation.



$$\begin{array}{rcl}
 \text{Op2} & = & -x, \quad y+\frac{1}{2}, \quad -z \\
 -\text{Op1} & = & -(x, \quad y, \quad z) \\
 \hline
 u & = & -2x, \quad \frac{1}{2}, \quad w = -2z
 \end{array}$$

$$\begin{array}{rcl}
 \text{Op1} & = & x, \quad y, \quad z \\
 -\text{Op2} & = & -(-x, \quad y+\frac{1}{2}, \quad -z) \\
 \hline
 u & = & 2x, \quad -\frac{1}{2}, \quad w = 2z
 \end{array}$$

In what planes do we expect difference Patterson peaks in $P2_12_12$?

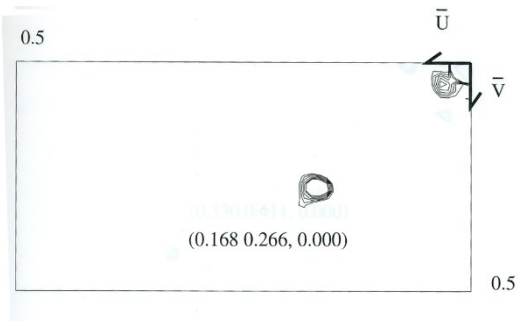
- (1) x , y , z
- (2) $-x$, $-y$, z
- (3) $-x+1/2$, $y+1/2$, $-z$
- (4) $x+1/2$, $-y+1/2$, $-z$

a) $w=0$

~~b) $w=1/2$~~

c) $v=1/2$

d) $u=1/2$



$$\begin{array}{l} 1) \quad X, \quad Y, \quad Z \\ 2) - (-X, \quad -Y, \quad Z) \\ \hline u=2x, \quad v=2y, \quad w=0 \end{array}$$

$$\begin{array}{l} u=2x \\ 0.168=2x \\ \mathbf{0.084=x} \end{array}$$

$$\begin{array}{l} v=2y \\ 0.266=2y \\ \mathbf{0.133=y} \end{array}$$

$$\begin{array}{l} 2) \quad -X, \quad -Y, \quad Z \\ 1) - (X, \quad Y, \quad Z) \\ \hline u=-2x, v=-2y, \quad w=0 \end{array}$$

$$\begin{array}{l} u=-2x \\ 0.168=-2x \\ \mathbf{-0.084=x} \end{array}$$

$$\begin{array}{l} v=-2y \\ 0.266=-2y \\ \mathbf{-0.133=y} \end{array}$$

$$\begin{array}{l} 3) \quad -x+\frac{1}{2} \quad y+\frac{1}{2} \quad -z \\ 4) - (x+\frac{1}{2} \quad -y+\frac{1}{2} \quad -z) \\ \hline u=-2x, \quad v=2y, \quad w=0 \end{array}$$

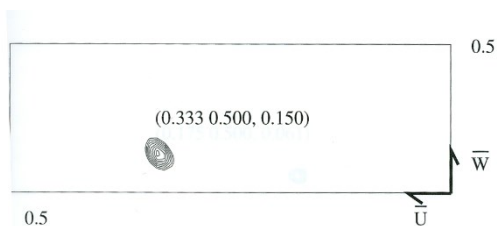
$$\begin{array}{l} u=-2x \\ 0.168=-2x \\ \mathbf{-0.084=x} \end{array}$$

$$\begin{array}{l} v=2y \\ 0.266=2y \\ \mathbf{0.133=y} \end{array}$$

$$\begin{array}{l} 4) \quad x+\frac{1}{2} \quad -y+\frac{1}{2} \quad -z \\ 3) - (-x+\frac{1}{2} \quad y+\frac{1}{2} \quad -z) \\ \hline u=2x, \quad v=-2y, \quad w=0 \end{array}$$

$$\begin{array}{l} u=2x \\ 0.168=2x \\ \mathbf{0.084=x} \end{array}$$

$$\begin{array}{l} v=-2y \\ 0.266=-2y \\ \mathbf{0.133=y} \end{array}$$



$$\begin{array}{l} 1) \quad X, \quad Y, \quad Z \\ 3) - (\frac{1}{2}X, \quad \frac{1}{2}Y, \quad -Z) \\ \hline u=2x-\frac{1}{2}, v=-\frac{1}{2}, w=2z \end{array}$$

$$\begin{array}{l} u=2x-\frac{1}{2} \\ 0.333=2x-\frac{1}{2} \\ 0.833=2x \\ \mathbf{0.416=x} \end{array}$$

$$\begin{array}{l} w=2z \\ 0.150=2z \\ \mathbf{0.075=z} \end{array}$$

$$\begin{array}{l} 3) \quad \frac{1}{2}X, \quad \frac{1}{2}Y, \quad -Z \\ 1) - (X, \quad Y, \quad Z) \\ \hline u=-2x+\frac{1}{2}, v=+\frac{1}{2}, w=-2z \end{array}$$

$$\begin{array}{l} u=-2x+\frac{1}{2} \\ 0.333=-2x+\frac{1}{2} \\ -0.167=-2x \\ \mathbf{0.084=x} \end{array}$$

$$\begin{array}{l} w=-2z \\ 0.150=-2z \\ \mathbf{-0.075=z} \end{array}$$

$$\begin{array}{l} 2) \quad -x \quad -y \quad z \\ 4) - (x+\frac{1}{2} \quad -y+\frac{1}{2} \quad -z) \\ \hline u=-2x-\frac{1}{2}, \quad v=-\frac{1}{2}, w=2z \end{array}$$

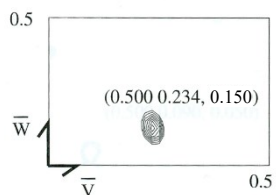
$$\begin{array}{l} u=-2x+\frac{1}{2} \\ 0.333=-2x-\frac{1}{2} \\ 0.833=-2x \\ \mathbf{-0.416=x} \end{array}$$

$$\begin{array}{l} w=2z \\ 0.150=2z \\ \mathbf{0.075=z} \end{array}$$

$$\begin{array}{l} 4) \quad x+\frac{1}{2} \quad -y+\frac{1}{2} \quad -z \\ 2) - (-x \quad -y \quad z) \\ \hline u=2x+\frac{1}{2}, \quad v=+\frac{1}{2}, w=-2z \end{array}$$

$$\begin{array}{l} u=2x+\frac{1}{2} \\ 0.333=2x+\frac{1}{2} \\ -0.167=2x \\ \mathbf{-0.084=x} \end{array}$$

$$\begin{array}{l} w=-2z \\ 0.150=-2z \\ \mathbf{-0.075=z} \end{array}$$



$$\begin{array}{l} 1) \quad X, \quad Y, \quad Z \\ 4) - (\frac{1}{2}X, \quad \frac{1}{2}Y, \quad -Z) \\ \hline u=-\frac{1}{2}, \quad v=2y-\frac{1}{2}, \quad w=2z \end{array}$$

$$\begin{array}{l} v=2y-\frac{1}{2} \\ 0.234=2y-\frac{1}{2} \\ 0.734=2y \\ \mathbf{0.367=y} \end{array}$$

$$\begin{array}{l} w=2z \\ 0.150=2z \\ \mathbf{0.075=z} \end{array}$$

$$\begin{array}{l} 4) \quad \frac{1}{2}X, \quad \frac{1}{2}Y, \quad -Z \\ 1) - (X, \quad Y, \quad Z) \\ \hline u=+\frac{1}{2}, \quad v=-2y+\frac{1}{2}, w=-2z \end{array}$$

$$\begin{array}{l} v=-2y+\frac{1}{2} \\ 0.234=-2y+\frac{1}{2} \\ -0.266=-2y \\ \mathbf{0.133=y} \end{array}$$

$$\begin{array}{l} w=-2z \\ 0.150=-2z \\ \mathbf{-0.075=z} \end{array}$$

$$\begin{array}{l} 2) \quad -x \quad -y \quad z \\ 3) - (\frac{1}{2}X, \quad \frac{1}{2}Y, \quad -Z) \\ \hline u=-\frac{1}{2}, v=-2y-\frac{1}{2}, \quad w=2z \end{array}$$

$$\begin{array}{l} v=-2y-\frac{1}{2} \\ 0.234=-2y-\frac{1}{2} \\ 0.734=-2y \\ \mathbf{-0.367=y} \end{array}$$

$$\begin{array}{l} w=2z \\ 0.150=2z \\ \mathbf{0.075=z} \end{array}$$

$$\begin{array}{l} 3) \quad \frac{1}{2}X, \quad \frac{1}{2}Y, \quad -Z \\ 2) - (-x \quad -y \quad z) \\ \hline u=+\frac{1}{2}, v=2y+\frac{1}{2}, w=-2z \end{array}$$

$$\begin{array}{l} v=2y+\frac{1}{2} \\ 0.234=2y+\frac{1}{2} \\ -0.266=2y \\ \mathbf{-0.133=y} \end{array}$$

$$\begin{array}{l} w=-2z \\ 0.150=-2z \\ \mathbf{-0.075=z} \end{array}$$

u	v	w
0.500	0.460	0.240

$$\begin{array}{r} 4) \quad \frac{1}{2}y \quad \frac{1}{2}x \quad \frac{1}{4}z}{5) - \left(\frac{y}{2} \quad \frac{x}{2} \quad -\frac{z}{4} \right)} \\ \hline u = \frac{1}{2}y, \quad v = \frac{1}{2}x, \quad w = \frac{1}{4}z \end{array}$$

$$\begin{array}{r} 3) \quad \frac{1}{2} - y \qquad \frac{1}{2} + x \qquad \frac{3}{4} + z \\ 6) - \left(\begin{array}{ccc} -y & -x & \frac{1}{2} - z \end{array} \right) \\ \hline u = \frac{1}{2}, \quad v = \frac{1}{2} + 2x, \quad w = \frac{1}{4} + 2z \end{array}$$

$$\begin{array}{r} 2) \quad -x \quad -y \quad \frac{1}{2}z \\ 7) - (\frac{1}{2}x \quad \frac{1}{2}y \quad \frac{3}{4}z) \\ \hline u = -\frac{1}{2}, \quad v = -\frac{1}{2} - 2y, \quad w = -\frac{1}{4} + 2z \end{array}$$

$$\begin{array}{r} 1) \quad \quad \quad x \quad \quad \quad y \quad \quad \quad z \\ 8) - (1/2x \quad \quad 1/2y \quad \quad 1/4z) \\ \hline u = -1/2, \quad v = -1/2 + 2y, \quad w = -1/4 + 2z \end{array}$$

Plug in v, solve for x:

$$0.460 = \frac{1}{2} - 2x$$
$$-0.040 = -2x$$
$$+0.020 = x$$

Plug in v, solve for x:

$$0.460 = \frac{1}{2} + 2x$$
$$-0.040 = 2x$$
$$-0.020 = x$$

Plug in v, solve for y:

$$0.460 = -\frac{1}{2} - 2y$$
$$0.960 = -2y$$
$$-0.480 = y$$

Plug in v, solve for y:

$$0.460 = -\frac{1}{2} + 2y$$
$$0.960 = 2y$$
$$+0.480 = y$$

Plug in w , solve for z :

$$0.240 = \frac{1}{4} + 2z$$
$$-0.010 = 2z$$
$$-0.005 = z$$

Plug in w, solve for z:

$$0.240 = \frac{1}{4} + 2z$$
$$-0.010 = 2z$$
$$-0.005 = z$$

Plug in w, solve for z:

$$0.240 = -\frac{1}{4} + 2z$$
$$0.490 = 2z$$
$$+0.245 = z$$

Plug in w, solve for z:

$$0.240 = -\frac{1}{4} + 2z$$
$$0.490 = 2z$$
$$+0.245 = z$$

[illegible]
$$-Y, \quad X, \quad 1/4+Z$$

u v w
0.180 0.220 0.250

$$\begin{array}{rcl} 2) & -x & -y & \frac{1}{2}+z \\ 4) & -(\frac{1}{2}+y & \frac{1}{2}-x & \frac{1}{4}+z) \\ \hline & u=-\frac{1}{2}-x-y, & v=-\frac{1}{2}+x-y, & w=\frac{1}{4} \end{array}$$

$$\begin{array}{rcl} 1) & x & y & z \\ 3) & -(\frac{1}{2}-y & \frac{1}{2}+x & \frac{3}{4}+z) \\ \hline & u=-\frac{1}{2}+x+y, & v=-\frac{1}{2}-x+y, & w=-\frac{3}{4} \end{array}$$

$$\begin{array}{rcl} 5) & y & x & -z \\ 7) & -(\frac{1}{2}-x & \frac{1}{2}+y & \frac{3}{4}-z) \\ \hline & u=-\frac{1}{2}+x+y, & v=-\frac{1}{2}+x-y, & w=-\frac{3}{4} \end{array}$$

$$\begin{array}{rcl} 6) & -y & -x & \frac{1}{2}-z \\ 8) & -(\frac{1}{2}+x & \frac{1}{2}-y & \frac{1}{4}-z) \\ \hline & u=-\frac{1}{2}-x-y, & v=-\frac{1}{2}-x+y, & w=\frac{1}{4} \end{array}$$

Take u-v, solve for x:

$$\begin{array}{r} u=-\frac{1}{2}-x-y \\ -(v=-\frac{1}{2}+x-y) \\ \hline u-v=-2x \\ (v-u)/2=x \end{array}$$

Plug in u & v, solve for x:

$$\begin{array}{r} (0.220-0.180)/2=x \\ (0.040)/2=x \\ \mathbf{0.020=x} \end{array}$$

Take u-v, solve for x:

$$\begin{array}{r} u=-\frac{1}{2}+x+y \\ -(v=-\frac{1}{2}-x+y) \\ \hline u-v=2x \\ (u-v)/2=x \end{array}$$

Plug in u & v, solve for x:

$$\begin{array}{r} (0.180-0.220)/2=x \\ (-0.040)/2=x \\ \mathbf{-0.020=x} \end{array}$$

Take u+v, solve for x:

$$\begin{array}{r} u=-\frac{1}{2}+x+y \\ +(v=-\frac{1}{2}+x-y) \\ \hline u+v=-1+2x \\ (u+v+1)/2=x \end{array}$$

Plug in u & v, solve for x:

$$\begin{array}{r} (0.180+0.220+1)/2=x \\ (1.400)/2=x \\ \mathbf{0.700=x} \end{array}$$

Take u+v, solve for x:

$$\begin{array}{r} u=-\frac{1}{2}-x-y \\ +(v=-\frac{1}{2}-x+y) \\ \hline u+v=-1-2x \\ -(u+v+1)/2=x \end{array}$$

Plug in u & v, solve for x:

$$\begin{array}{r} -(0.180+0.220-1)/2=x \\ -(-0.600)/2=x \\ \mathbf{0.300=x} \end{array}$$

Take u+v and solve for y:

$$\begin{array}{r} u=-\frac{1}{2}-x-y \\ +(v=-\frac{1}{2}+x-y) \\ \hline u+v=-1-2y \\ -(u+v+1)/2=y \end{array}$$

Plug in u & v, solve for y:

$$\begin{array}{r} -(0.180+0.220+1)/2=y \\ -(1.400)/2=y \\ \mathbf{-0.700=y} \end{array}$$

Take u+v and solve for y:

$$\begin{array}{r} u=-\frac{1}{2}+x+y \\ +(v=-\frac{1}{2}-x+y) \\ \hline u+v=-1+2y \\ (u+v+1)/2=y \end{array}$$

Plug in u & v, solve for y:

$$\begin{array}{r} (0.180+0.220+1)/2=y \\ (1.400)/2=y \\ \mathbf{0.700=y} \end{array}$$

Take u-v and solve for y:

$$\begin{array}{r} u=-\frac{1}{2}+x+y \\ -(v=-\frac{1}{2}+x-y) \\ \hline u-v=2y \\ (u-v)/2=y \end{array}$$

Plug in u & v, solve for y:

$$\begin{array}{r} (0.180-0.220)/2=y \\ -(0.040)/2=y \\ \mathbf{-0.020=y} \end{array}$$

Take u-v and solve for y:

$$\begin{array}{r} u=-\frac{1}{2}-x-y \\ -(v=-\frac{1}{2}-x+y) \\ \hline u-v=-2y \\ -(u-v)/2=y \end{array}$$

Plug in u & v, solve for y:

$$\begin{array}{r} -(0.180-0.220)/2=y \\ -(-0.040)/2=y \\ \mathbf{0.020=y} \end{array}$$

no	x	y	z	xt	yt	zt
4-5	0.020		0.995		+0.020	0.245
3-6	0.980		0.995			
2-7		0.520	0.245			
1-8		0.480	0.245			
2-4	0.020	0.300				
1-3	0.980	0.700				
5-7	0.700	0.020				

x	y	z	0.793022	0.509201	0.002329
-x	-y	z	0.206978	0.490799	0.002329
-y	x	z+1/4	0.490799	0.793022	0.252329
y	-x	z+1/4	0.509201	0.206978	0.252329
y	x	-z	0.509201	0.793022	0.997671
-y	-x	-z	0.490799	0.206978	0.997671
x	-y	-z+1/4	0.793022	0.490799	0.247671
-x	y	-z+1/4	0.206978	0.509201	0.247671

(1/2, 1/2, 0)					
x+1/2	y+1/2	z	0.293022	0.009201	0.002329
-x+1/2	-y+1/2	z	0.706978	0.990799	0.002329
-y+1/2	x+1/2	z+1/4	0.990799	0.293022	0.252329
y+1/2	-x+1/2	z+1/4	0.009201	0.706978	0.252329
y+1/2	x+1/2	-z	0.009201	0.293022	0.997671
-y+1/2	-x+1/2	-z	0.990799	0.706978	0.997671
x+1/2	-y+1/2	-z+1/4	0.293022	0.990799	0.247671
-x+1/2	y+1/2	-z+1/4	0.706978	0.009201	0.247671

(0, 0, 1/2)					
x	y	z+1/2	0.793022	0.509201	0.502329
-x	-y	z+1/2	0.206978	0.490799	0.502329
-y	x	z+3/4	0.490799	0.793022	0.752329
y	-x	z+3/4	0.509201	0.206978	0.752329
y	x	-z+1/2	0.509201	0.793022	0.497671
-y	-x	-z+1/2	0.490799	0.206978	0.497671
x	-y	-z+3/4	0.793022	0.490799	0.747671
-x	y	-z+3/4	0.206978	0.509201	0.747671

(1/2, 1/2, 1/2)						
x+1/2	y+1/2	z+1/2	0.293022	0.009201	0.502329	
-x+1/2	-y+1/2	z+1/2	0.706978	0.990799	0.502329	
-y+1/2	x+1/2	z+3/4	0.990799	0.293022	0.752329	
y+1/2	-x+1/2	z+3/4	0.009201	0.706978	0.752329	
y+1/2	x+1/2	-z+1/2	0.009201	0.293022	0.497671	
-y+1/2	-x+1/2	-z+1/2	0.990799	0.706978	0.497671	
x+1/2	-y+1/2	-z+3/4	0.293022	0.990799	0.747671	
-x+1/2	y+1/2	-z+3/4	0.706978	0.009201	0.747671	

[illegible]

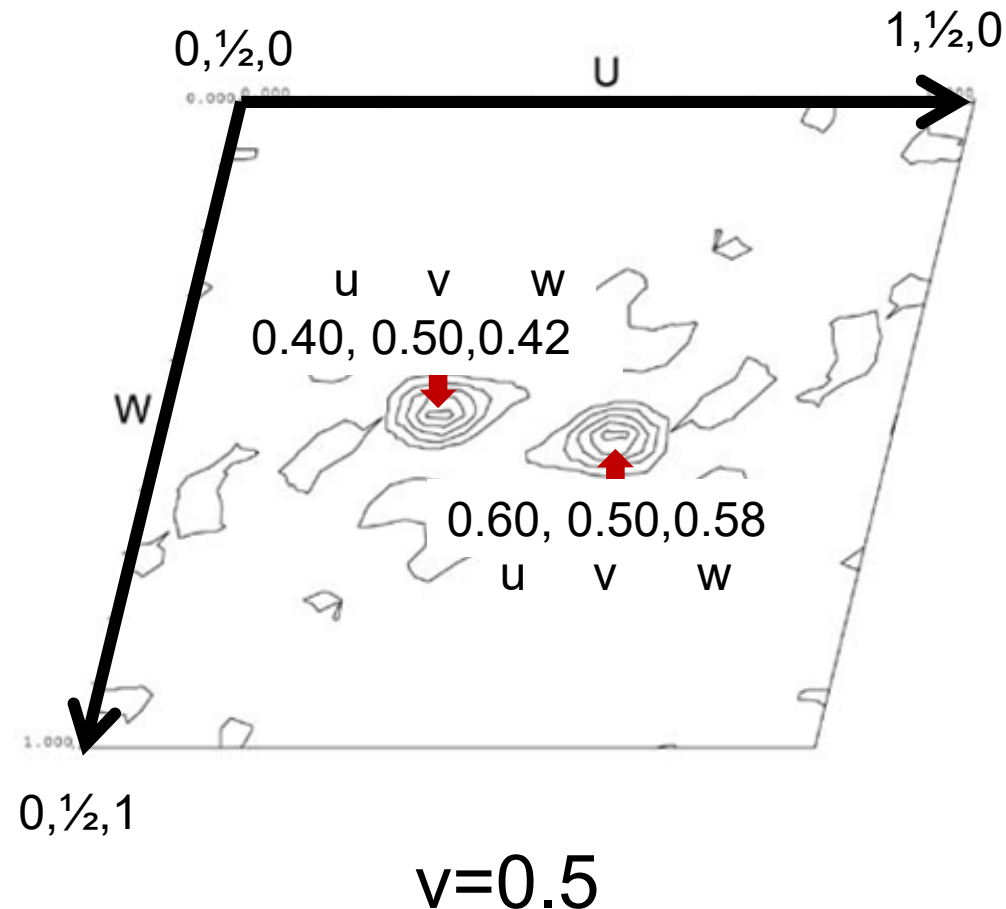
Determine the heavy atom substructure of Zn^{2+} -NNQQNY

- Zinc is the heavy atom.
- Difference Patterson map shows peaks from Zn.
- Space group $P2_1$
- Unit cell parameters
 $a=21.1 \text{ \AA}$ $b=4.8 \text{ \AA}$ $c=23.1 \text{ \AA}$
 $\alpha=90.0^\circ$ $\beta=103.0^\circ$ $\gamma=90.0^\circ$



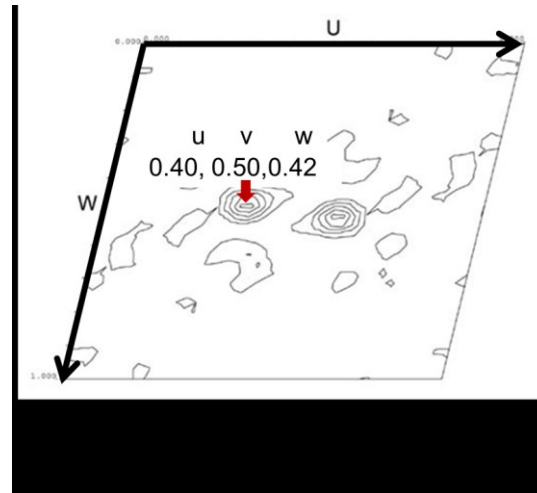
Difference Patterson map of $\text{Zn}^{2+}\text{NNQQNY}$

- Two strong peaks are visible in the difference Patterson map.
- The space group is $P2_1$.
- What are the coordinates of the zinc ions?

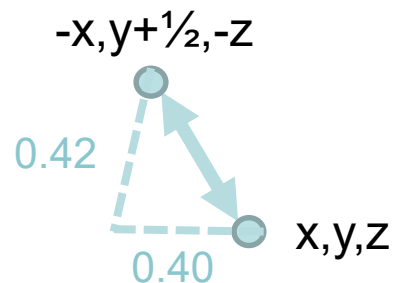
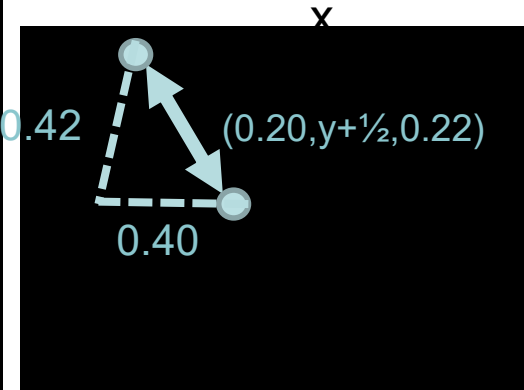


We can interpret this difference Patterson map using 2 basic concepts.

A difference Patterson peak with coordinates (u,v,w) , tells us that two atoms in the crystal are related by a vector with length u (along x), a length v (along y), and a length w (along z). In other words, the vector relating two atoms in the crystal has the magnitude and direction of a vector $\mathbf{u}, \mathbf{v}, \mathbf{w}$. So, the Patterson peak coordinates tell us the relative positions of the two atoms, but not the absolute positions of the atoms.



$(-0.20, y, -0.22)$



$$\begin{aligned} \text{Op2} &= -x, y+\frac{1}{2}, -z \\ -\text{Op1} &= -(x, y, z) \\ \hline u &= -2x, v = \frac{1}{2}, w = -2z \\ 0.40 &= -2x & 0.42 &= -2z \\ -0.20 &= x & -0.22 &= z \end{aligned}$$

To determine the absolute positions of the atoms, we need to know the space group symmetry operator that relates the two atoms at the tips of the vector, u, v, w . If we can attribute the two atoms to space group symmetry operators, we can equate the difference between operators to u, v, w and solve for x, y, z .

$P2_1$ Symmetry operators

$$(1) x, y, z \quad (2) -x, y+\frac{1}{2}, -z$$

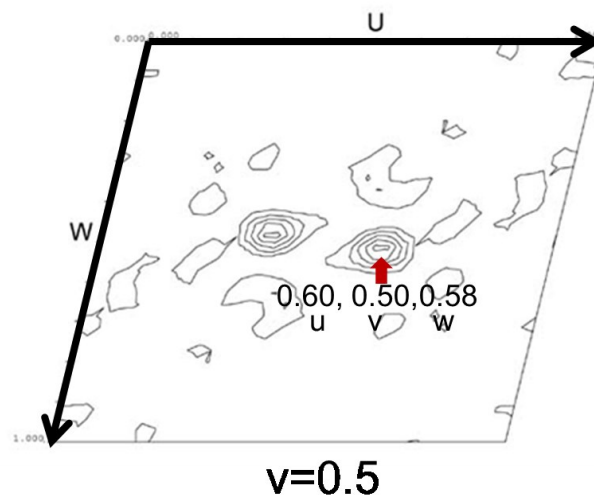
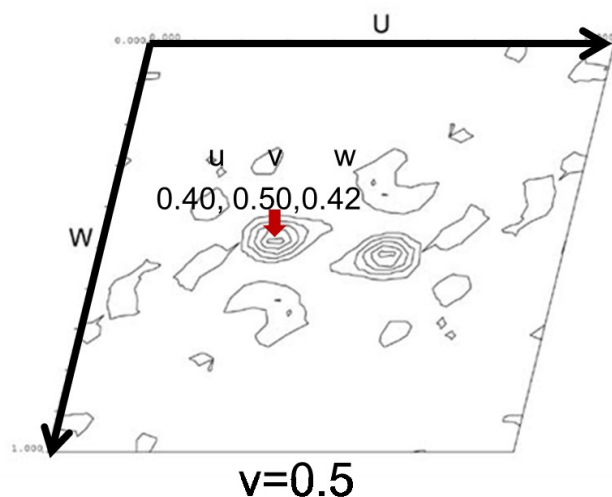
Numerically distinct, but equally valid values of x,y,z could be obtained.

We could have subtracted the symmetry operators in a different order.

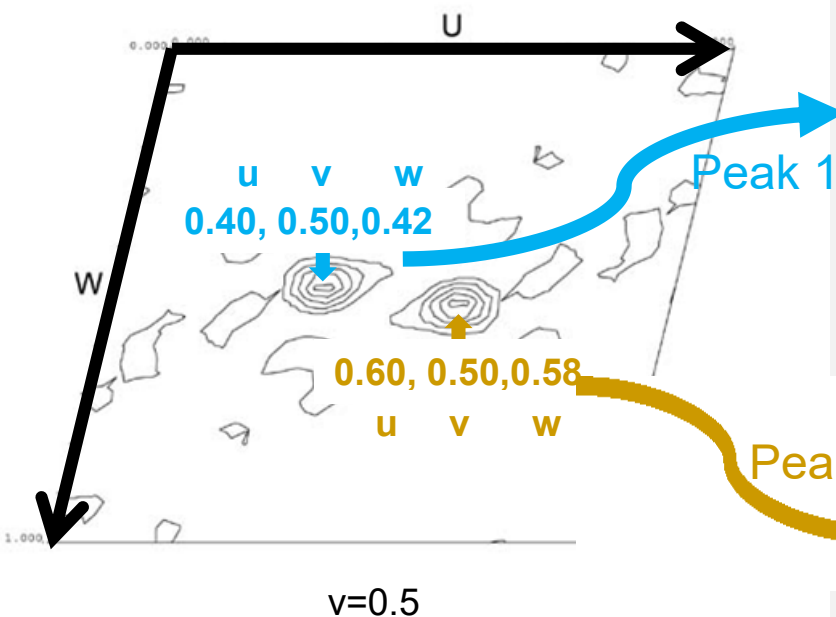
$$\begin{array}{rcl} \text{Op2} & = & -x, \quad y + \frac{1}{2}, \quad -z \\ -\text{Op1} & = & -(x, \quad y, \quad z) \\ \hline u & = & -2x, \quad \frac{1}{2}, \quad w = -2z \end{array}$$

$$\begin{array}{rcl} \text{Op1} & = & x, \quad y, \quad z \\ -\text{Op2} & = & -(-x, \quad y + \frac{1}{2}, \quad -z) \\ \hline u & = & 2x, \quad -\frac{1}{2}, \quad w = 2z \end{array}$$

We could have chosen to use a different Patterson peak (u,v,w)



Solve for x,z coordinates of Zn ion.



Op2-Op1

$$\begin{array}{ll} x = -u/2 & z = -w/2 \\ x = - & /2 \quad z = - & /2 \\ x = -0.20 & z = -0.21 \\ \boxed{x = +0.80} & \boxed{z = +0.79} \end{array}$$

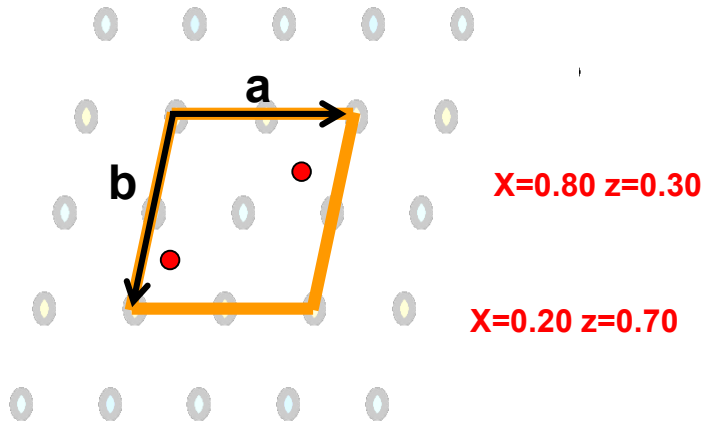
Op1-Op2

$$\begin{array}{ll} x = u/2 & z = w/2 \\ x = & /2 \quad z = & /2 \\ \boxed{x = 0.20} & \boxed{z = 0.21} \end{array}$$

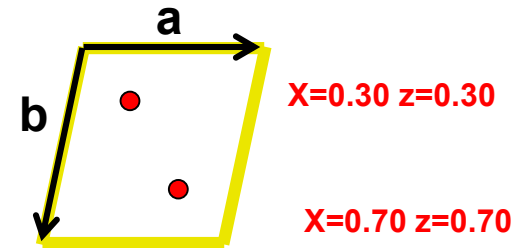
You are allowed to add or subtract 1 from any coordinate dimension, x, y or z. Such operations shift the atom unit cell increments. Why do it? positive numbers are less cumbersome than negative numbers.

The four Zn coordinate solutions are all valid.
They differ by origin shifts. Compare unit cells

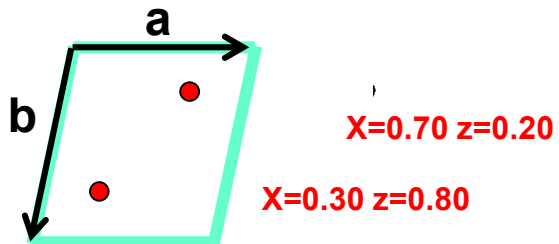
Choice 1



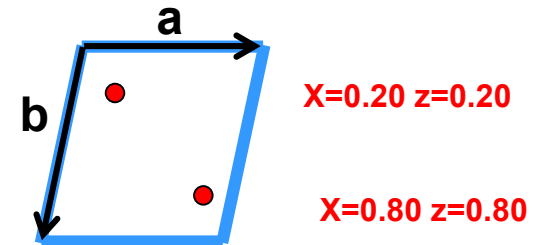
Choice 2



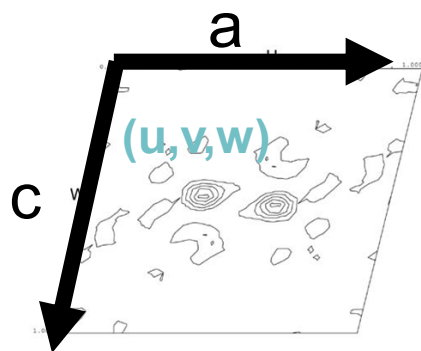
Choice 3



Choice 4

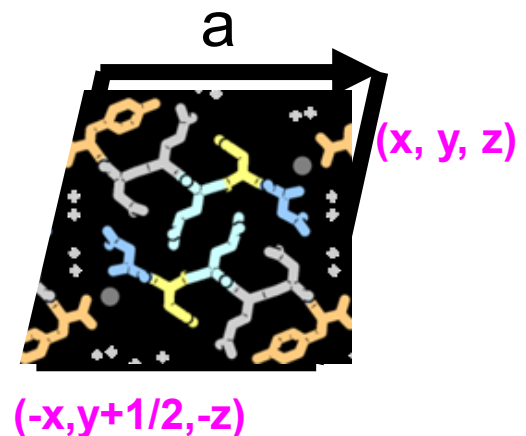


Lesson: symmetry operators are the bridge between atomic coordinates in the crystal and Patterson peaks



Difference Patterson Map

$$\begin{array}{r} (-x, y+1/2, -z) \\ -(x, y, z) \\ \hline (-2x, 1/2, -2z) \\ u \quad v \quad w \end{array}$$

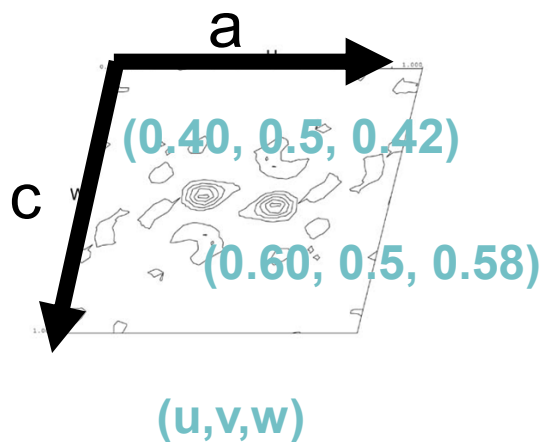


Crystal Structure

Patterson prediction $u=-2x, w=-2z$

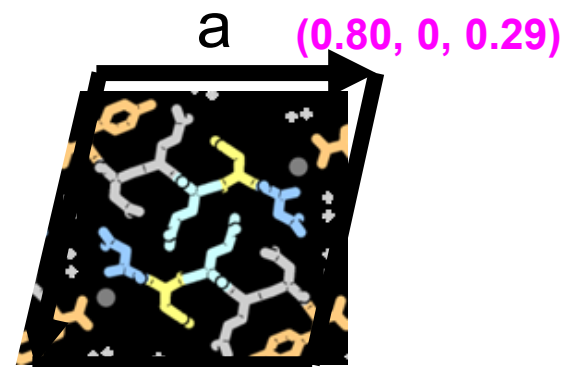
Heavy atom structure determination $x=-u/2 \quad z=-w/2$

Lesson: Check that your x,y,z can predict u,v,w.
It's easy to make an algebraic error.



Difference Patterson Map

$$\begin{array}{r}
 (-x, y+1/2, -z) \\
 -(x, y, z) \\
 \hline
 (-2x, 1/2, -2z) \\
 u \quad v \quad w
 \end{array}$$



Crystal Structure



$$u = -2x$$

$$u = -2 \cdot 0.80 = -1.6 = 0.4$$

$$w = -2z$$

$$w = -2 \cdot 0.29 = -0.58 = 0.42$$

DNA polymerase β

Pt derivative

$P2_12_12$

4 symmetry operators

(1) x, y, z

(2) $-x, -y, z$

(3) $-x + 1/2, y + 1/2, -z$

(4) $x + 1/2, -y + 1/2, -z$

Crystal Structure of Rat DNA Polymerase β : Evidence for a Common Polymerase Mechanism

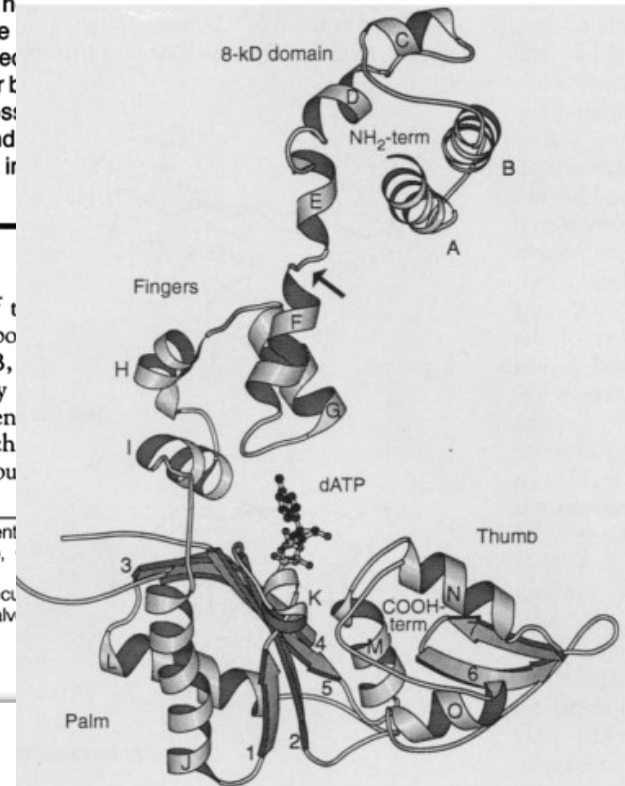
Michael R. Sawaya, Huguet Pelletier, Amalendra Kumar,
Samuel H. Wilson, Joseph Kraut

Structures of the 31-kilodalton catalytic domain of rat DNA polymerase β (pol β) and the whole 39-kilodalton enzyme were determined at 2.3 and 3.6 angstrom resolution, respectively. The 31-kilodalton domain is composed of fingers, palm, and thumb subdomains arranged to form a DNA binding channel reminiscent of the polymerase domains of the Klenow fragment of *Escherichia coli* DNA polymerase I, HIV-1 reverse transcriptase, and bacteriophage T7 RNA polymerase. The arrangement within structurally similar polymerases have maintained, or possibly mechanism. The location of Mn^{2+} and the role of the invariant aspartates in binding.

DNA polymerase β (pol β) is one of the four recognized DNA-directed DNA polymerases of the eukaryotic nucleus: α , β , γ , and δ . It has been studied primarily in vertebrates but homologs have also recently been discovered in lower eukaryotes such as yeast (1) and trypanosomes (2). Although

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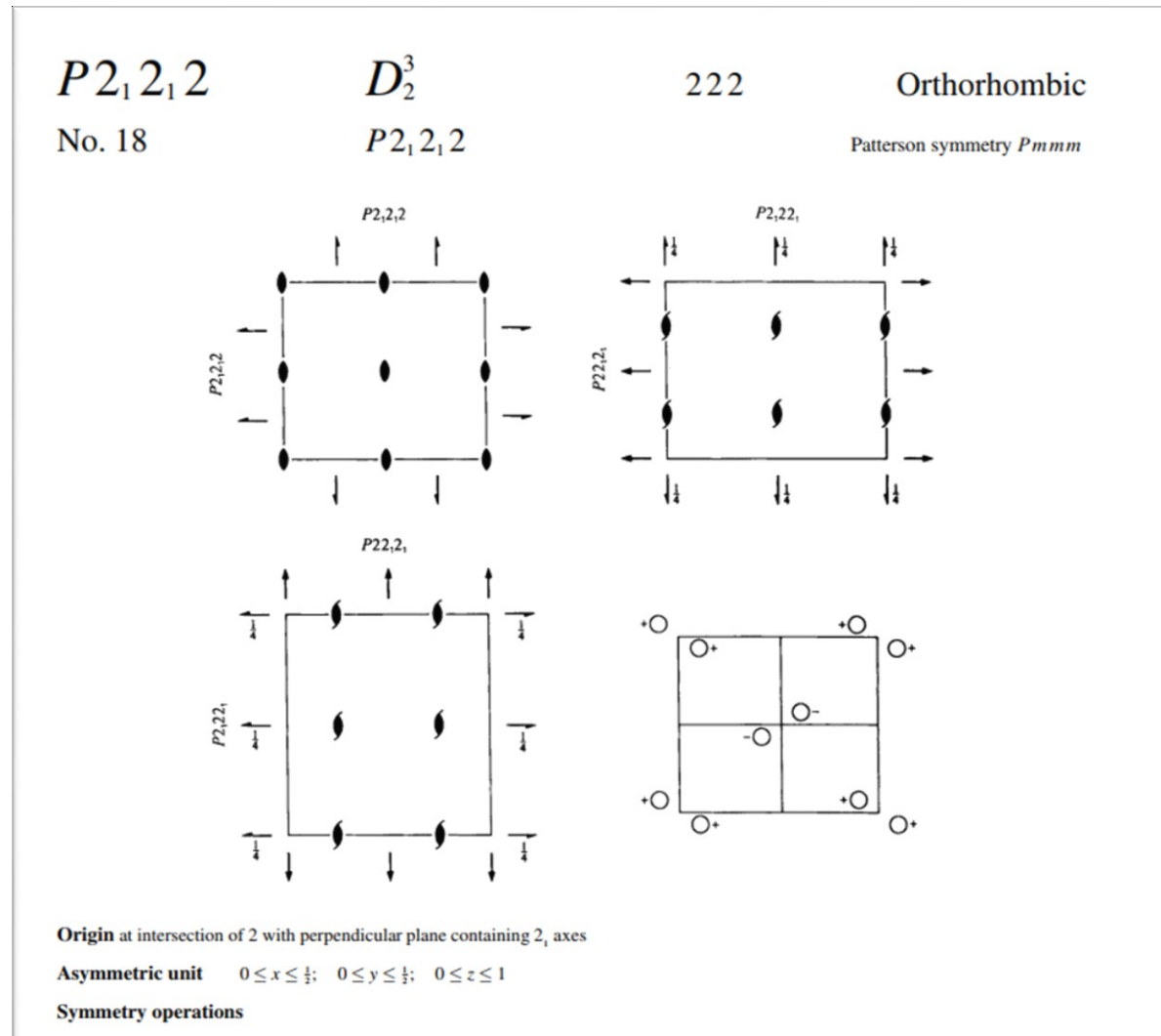


Symmetry operators are listed in the Int'l Tables of Crystallography Vol A.

Symmetry operators

- (1) x, y, z
- (2) $-x, -y, z$
- (3) $-x+1/2, y+1/2, -z$
- (4) $x+1/2, -y+1/2, -z$

- What symmetry axes are present?
- How are the axes oriented?



Pt derivative DNA polymerase β

$P2_12_12$

- (1) x, y, z (reference)
- (2) $-x, -y, z$ (2-fold around z)
- (3) $-x + 1/2, y + 1/2, -z$ (2_1 around y)
- (4) $x + 1/2, -y + 1/2, -z$ (2_1 around x)

Illustrate with
asymmetric unit=
Right hand

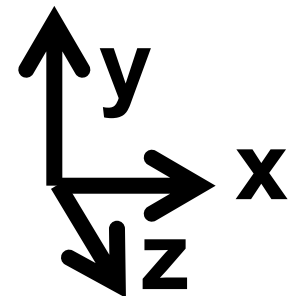


(3) $-x + 1/2, y + 1/2, -z$



(4) $x + 1/2, -y + 1/2, -z$

How many Patterson peak are expected for a
single heavy atom site in $P2_12_12$ asymmetric unit?
List the difference vectors expressions in $P2_12_12$.



Dear Mikey 2022,

This lecture in 2021 was a disaster. You went 5 minutes over. Nobody asked questions. There was confusion about why you don't have a y coordinate in P21. I am not sure if people understood the symmetry display with hands. Duilio says it is difficult to see the symmetry relationship among the hands. Need different colors or animate with a movie to view from different perspectives. I think the outline that I wrote was clear. Check it out. I just didn't have time to make the presentation align well with the outline. I suggest spending time to alter the slides to match the outline. Could help to draw symmetry operators for screw axes on slide 4. It always take such a long time to explain the checking procedure at the end. People don't understand that our map has a limited extent of one asymmetric unit, and the prediction we make often falls outside the asymmetric unit, so we have to apply unit cell translations and Patterson symmetry operations to map our prediction to the asymmetric unit cell. Maybe you can make a slide to illustrate that. People want to see procedures illustrated for when you get incorrect hand. Maybe skip manual checking step and just do `checkpatterson.csh`. Love- Mikey 2021

Our goal is to determine the position of the heavy atom(s) with respect to the unit cell origin (i.e. coordinates x,y,z). We are provided a few clues.

A difference Patterson map reveals the relative positions of pairs of atoms in the unit cell –i.e. vectors. The vectors (having x , y , and z components) between atoms are encoded as the coordinates of the difference Patterson peak (u,v,w).

Symmetry operators provide a formula for converting this vector u,v,w into coordinates (x,y,z). How does this work?

Symmetry operators describe the general positions of atoms in a unit cell. For example, in $P21212$, there are four symmetry operators.

(1) x, y, z

(2) $-x, -y, z$

(3) $-x+1/2, y+1/2, -z$

(4) $x+1/2, -y+1/2, -z$

Vectors between atoms may be expressed as the differences between these general positions. For example, $(x,y,z) - (-x,-y,z)$ is a vector between an atom at position x,y,z and the position $-x,-y,z$. In other words, $u=2x$, $v=2y$, $w=0$. We plug in values of u,v,w to find x,y,z .

Be careful to match each difference Patterson peak with the appropriate pair of symmetry operators, or else values of x,y,z will be incorrect.

The position of the difference Patterson peak on Harker sections offers a clue to choosing the appropriate pair of symmetry operators. For example, a difference Patterson peak on the $w=0$ plane might be attributed to $(x,y,z) - (-x,-y,z)$, because $w=0$ is consistent with difference between these two symmetry operators giving $w=0$.