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, \( \alpha_{hkl} \), 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:
- $a=120.5 \text{ Å}$, $b=63.5 \text{ Å}$, $c=38.2 \text{ Å}$, $\alpha=\beta=\gamma=90^\circ$
- $0.168 \times 120.5 \text{ Å} = 20.2 \text{ Å}$
- $0.266 \times 63.5 \text{ Å} = 16.9 \text{ Å}$
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\textsubscript{1}2\textsubscript{1}2\textsubscript{1}, there are four symmetry operators.
  1. \(x, y, z\)
  2. \(-x, -y, z\)
  3. \(-x + \frac{1}{2}, y + \frac{1}{2}, -z\)
  4. \(x + \frac{1}{2}, -y + \frac{1}{2}, -z\)
- 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:
  1. \(-0.1, -0.2, 0.3\)
  2. \(0.4, 0.7, -0.3\)
  3. \(0.5, 0.3, -0.3\)
Differences between symmetry equivalent positions equate Patterson vectors to the atomic coordinates.

For example, we have seen space group P2₁2₁2 has 4 symmetry equivalent positions:

1. \( x, \ y, \ z \)
2. \(-x, \ -y, \ z\)
3. \(-x+\frac{1}{2}, \ y+\frac{1}{2}, \ -z\)
4. \(x+\frac{1}{2}, \ -y+\frac{1}{2}, \ -z\)

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. \( x, \ y, \ z \)
2. \(-x, \ -y, \ z\)
\( u=2x, \ v=2y, \ w=0 \)

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

\[
\begin{align*}
0.168 &= 2x \\
0.084 &= x \\
0.266 &= 2y \\
0.133 &= y
\end{align*}
\]

Plug in \( u \) to solve for \( x \):
\[
0.168 = 2x \quad \Rightarrow \quad x = 0.084
\]

Plug in \( v \) to solve for \( y \):
\[
0.266 = 2y \quad \Rightarrow \quad y = 0.133
\]

The only remaining task is to determine the coordinate, \( z \).
What is the value of z?

1. X, Y, Z
2. -X, -Y, Z

\[ u = 2x, \quad v = 2y, \quad w = 0 \]

\[ a) \text{Zero} \]
\[ b) \ x/y \]
\[ c) \text{not specified by this map section.} \]
What is the value of z?

1. X, Y, Z
2. -X, -Y, Z
   u=2x, v=2y, w=0

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\textsubscript{1}2\textsubscript{1}2. How many?

<table>
<thead>
<tr>
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<th>1</th>
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<th>3</th>
<th>4</th>
</tr>
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<tbody>
<tr>
<td>x y z</td>
<td>1-1</td>
<td>2-1</td>
<td>3-1</td>
<td>4-1</td>
</tr>
<tr>
<td>-x -y z</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-x+\frac{1}{2} y+\frac{1}{2} -z</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>x+\frac{1}{2} -y+\frac{1}{2} -z</td>
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</tbody>
</table>
How many of these peaks are off-origin?

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<tbody>
<tr>
<td><strong>Symmetry ops</strong></td>
<td>x y z</td>
<td>-x -y z</td>
<td>-x+1/2 y+1/2 -z</td>
<td>x+1/2 -y+1/2 -z</td>
</tr>
<tr>
<td>1</td>
<td>x y z</td>
<td>x y z</td>
<td>-x -y z</td>
<td>-x+1/2 y+1/2 -z</td>
</tr>
<tr>
<td>2</td>
<td>-x -y z</td>
<td>x y z</td>
<td>-x -y z</td>
<td>-x+1/2 y+1/2 -z</td>
</tr>
<tr>
<td>3</td>
<td>-x+1/2 y+1/2 -z</td>
<td>x y z</td>
<td>x y z</td>
<td>x+1/2 -y+1/2 -z</td>
</tr>
<tr>
<td>4</td>
<td>x+1/2 -y+1/2 -z</td>
<td>x y z</td>
<td>-x -y z</td>
<td>-x+1/2 y+1/2 -z</td>
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</tbody>
</table>
In what planes do we expect difference Patterson peaks in P2₁2₁2?
In what planes do we expect difference Patterson peaks in \( P2_12_12 \)?

<table>
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</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( x )</td>
<td>( y )</td>
<td>( z )</td>
<td>( -x )</td>
</tr>
<tr>
<td>1 ( x \ y \ z )</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-2( x )</td>
</tr>
<tr>
<td>2 ( -x \ -y \ z )</td>
<td>2( x )</td>
<td>2( y )</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>3 ( -x+\frac{1}{2} \ y+\frac{1}{2} \ -z )</td>
<td>2( x-\frac{1}{2} )</td>
<td>-( \frac{1}{2} )</td>
<td>2( z )</td>
<td>-( \frac{1}{2} )</td>
</tr>
<tr>
<td>4 ( x+\frac{1}{2} \ -y+\frac{1}{2} \ -z )</td>
<td>-( \frac{1}{2} )</td>
<td>2( y-\frac{1}{2} )</td>
<td>2( z )</td>
<td>-2( x-\frac{1}{2} )</td>
</tr>
</tbody>
</table>
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?

1. $X, Y, Z$
2. $-X, -Y, Z$
   \[ u=2x, v=2y, w=0 \]
3. $\frac{1}{2}-X, \frac{1}{2}+Y, -Z$
   \[ u=2x-\frac{1}{2}, v=-\frac{1}{2}, w=2z \]
4. $\frac{1}{2}+X, \frac{1}{2}+Y, -Z$
   \[ u=-\frac{1}{2}, v=2y-\frac{1}{2}, w=2z \]

**d) They are all equally likely.**
Which of these difference vectors is likely to correspond to the difference Patterson peak shown here?

\[ u = 2x, \quad v = 2y, \quad w = 0 \]

\[ \frac{1}{2} - x, \frac{1}{2} + y, -z \]

\[ u = 2x - \frac{1}{2}, \quad v = -\frac{1}{2}, \quad w = 2z \]
Harker Section $v = \frac{1}{2}$

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

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?

\[
\begin{align*}
0.168 &= 2x \\
0.084 &= x \\
0.266 &= 2y \\
0.133 &= y \\
0.333 &= 2x - 1/2 \\
0.833 &= 2x \\
0.416 &= x \\
0.150 &= 2z \\
0.075 &= z
\end{align*}
\]

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

x, y, z
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 $P2_{1\overline{2}}\overline{1}2$. 
Cheshire symmetry allows either choice of x,y,z values

| Combo 1 | x(from w=0)=0.084, y(from w=0)=0.133, z(from v=½)=0.075 |
| Combo 2 | x(from v=½)=0.416, y(from w=0)=0.133, z(from v=½)=0.075 |

1. X, Y, Z
2. -X, -Y, Z
3. -X, Y, -Z
4. X, -Y, -Z
5. -X, -Y, -Z
6. X, Y, Z
7. X, -Y, Z
8. -X, Y, Z
9. 1/2+X, Y, Z
10. 1/2-X, -Y, Z
11. 1/2-X, Y, -Z
12. 1/2+X, -Y, -Z
13. 1/2-X, -Y, -Z
14. 1/2+X, Y, -Z
15. 1/2+X, -Y, Z
16. 1/2-X, Y, Z

1) X= 0.084, y= 0.133, z= 0.075

33. 1/2+X, 1/2+Y, Z
34. 1/2-X, 1/2-Y, Z
35. 1/2-X, 1/2+Y, -Z
36. 1/2+X, 1/2-Y, -Z
37. 1/2-X, 1/2-Y, -Z
38. 1/2+X, 1/2+Y, -Z
39. 1/2+X, 1/2-Y, Z
40. 1/2-X, 1/2+Y, Z

25. X= 0.584, y= 0.133, z= 0.075
26. X= 0.416, y= 0.133, z= 0.075
27. X= 0.416, y= 0.367, z= 0.075
28. X= 0.584, y= 0.367, z= 0.075
29. X= 0.584, y= 0.367, z= 0.075
30. X= 0.584, y= 0.367, z= 0.075
31. X= 0.584, y= 0.367, z= 0.075
32. X= 0.584, y= 0.367, z= 0.075
Check your algebra by predicting \((u,v,w)\) of the remaining Patterson peak

Combo 1 \(x=0.084, y=0.133, z=0.075\)

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<tr>
<td>(x\ y\ z)</td>
<td>(-x\ -y\ z)</td>
<td>(-x+\frac{1}{2}\ y+\frac{1}{2}\ -z)</td>
<td>(x+\frac{1}{2}\ -y+\frac{1}{2}\ -z)</td>
<td></td>
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</tbody>
</table>

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

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

\(v = -0.266 + \frac{1}{2}\)

\(v = 0.234\)

\(w = -2z\)

\(w = -2(0.075)\)

\(w = -0.140\)

\(U = \frac{1}{2}\)

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 \(x=0.084, y=0.133, z=0.075\)

\[
\begin{align*}
U &= \frac{1}{2} \\
v &= -2y + \frac{1}{2} \\
w &= -2z
\end{align*}
\]

\[
\begin{align*}
U &= \frac{1}{2} \\
v &= -2(0.133) + \frac{1}{2} \\
w &= -2(0.075)
\end{align*}
\]

\[
\begin{align*}
U &= \frac{1}{2} \\
v &= 0.234 \\
w &= -0.140
\end{align*}
\]
Is the prediction $(\frac{1}{2}, 0.234, -0.140)$ a match with recorded peak $(\frac{1}{2}, 0.234, 0.140)$?

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 P4₃2₁₂

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

1. \( x, y, z \)
2. \( x, y, \frac{1}{2} + z \)
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. \( y, x, \frac{1}{2} - z \)
8. \( y, x, \bar{z} \)

8*8=64 Patterson peaks
8 peaks are at 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
# Table of Patterson Difference Vectors (U,V,W)

## 8 symmetry operators in space group P4,2,2

<table>
<thead>
<tr>
<th>Operator</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>x</td>
<td>y</td>
<td>z</td>
</tr>
<tr>
<td>2</td>
<td>-x</td>
<td>-y</td>
<td>1/2 + z</td>
</tr>
<tr>
<td>3</td>
<td>1/2 - y</td>
<td>1/2 + x</td>
<td>3/4 + z</td>
</tr>
<tr>
<td>4</td>
<td>1/2 + y</td>
<td>1/2 - x</td>
<td>1/4 + z</td>
</tr>
<tr>
<td>5</td>
<td>y</td>
<td>x</td>
<td>- z</td>
</tr>
<tr>
<td>6</td>
<td>- y</td>
<td>- x</td>
<td>1/2 - z</td>
</tr>
<tr>
<td>7</td>
<td>1/2 - x</td>
<td>1/2 + y</td>
<td>3/4 - z</td>
</tr>
<tr>
<td>8</td>
<td>1/2 + x</td>
<td>1/2 - y</td>
<td>1/4 - z</td>
</tr>
</tbody>
</table>

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<td>-y</td>
<td>1/2 + z</td>
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<tr>
<td>3</td>
<td>1/2 - y</td>
<td>1/2 + x</td>
<td>3/4 + z</td>
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<td>4</td>
<td>1/2 + y</td>
<td>1/2 - x</td>
<td>1/4 + z</td>
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<tr>
<td>5</td>
<td>y</td>
<td>x</td>
<td>- z</td>
</tr>
<tr>
<td>6</td>
<td>- y</td>
<td>- x</td>
<td>1/2 - z</td>
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<td>z</td>
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<tr>
<td>2</td>
<td>-x</td>
<td>-y</td>
<td>1/2 + z</td>
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<td>3</td>
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<td>1/2 + x</td>
<td>3/4 + z</td>
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<td>4</td>
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<td>1/2 - x</td>
<td>1/4 + z</td>
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<tr>
<td>5</td>
<td>y</td>
<td>x</td>
<td>- z</td>
</tr>
<tr>
<td>6</td>
<td>- y</td>
<td>- x</td>
<td>1/2 - z</td>
</tr>
<tr>
<td>7</td>
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<td>1/2 - y</td>
<td>1/4 - z</td>
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</table>
isomorphous difference Patterson map
\( u = 0.50 \)
isomorphous difference Patterson map

$u = 0.50$

Symmetry operator 3
-Symmetry operator 6

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

\[
\begin{array}{c}
0.500 \\
0.460 \\
0.240
\end{array}
\]
Plug in $v$, solve for $x$:

\[
v = \frac{1}{2} + 2x
\]

\[
0.460 = \frac{1}{2} + 2x
\]

\[
-0.040 = 2x
\]

\[
-0.020 = x
\]
Symmetry operator 3
-Symmetry operator 6

\[
\begin{bmatrix}
\frac{1}{2} - y & \frac{1}{2} + x & \frac{3}{4} + z \\
-(-y) & -x & \frac{1}{2} - z
\end{bmatrix}
\]

\[
u = \frac{1}{2}, \quad v = \frac{1}{2} + 2x, \quad w = \frac{3}{4} + 2z
\]

Plug in \( w \), solve for \( z \):

\[
v = \frac{1}{2} + 2x
\]

\[
0.460 = \frac{1}{2} + 2x
\]

\[
-0.040 = 2x
\]

\[
-0.020 = x
\]

Plug in \( v \), solve for \( x \):

\[
v = \frac{1}{2} + 2x
\]

\[
0.460 = \frac{1}{2} + 2x
\]

\[
-0.040 = 2x
\]

\[
-0.020 = x
\]
isomorphous difference Patterson map

W=0.25

u     v     w
0.180 0.220 0.250

u     v     w
0.180 0.220 0.250
Symmetry operator 2
-Symmetry operator 4

\[
\begin{align*}
2) & \quad -y & \quad \frac{1}{2} + z \\
4) & \quad \left(\frac{1}{2} + y, \quad \frac{1}{2} - x, \quad \frac{1}{4} + z\right) \\
\quad & \quad u = -\frac{1}{2} - x - y, \quad v = -\frac{1}{2} + x - y, \quad w = \frac{1}{4}
\end{align*}
\]
Symmetry operator 2
-Symmetry operator 4

\[
\begin{align*}
2) & \quad -x & -y & \frac{1}{2} + z \\
4) & \quad \left(\frac{1}{2} + y \quad \frac{1}{2} - x \quad \frac{1}{4} + z\right)
\end{align*}
\]

\[
\begin{align*}
u &= -\frac{1}{2} - x - y, & v &= -\frac{1}{2} + x - y, & w &= \frac{1}{4}
\end{align*}
\]

Plug in \( u \) and solve for \( x \).

\[
\begin{align*}
u &= -\frac{1}{2} - x - y \\
0.180 &= -\frac{1}{2} - x - y \\
0.680 &= -x - y
\end{align*}
\]
Symmetry operator 2
-Symmetry operator 4

2) \(-x \quad -y \quad \frac{1}{2}+z\)
4) \(-\left(\frac{1}{2}+y \quad \frac{1}{2}-x \quad \frac{1}{4}+z\right)\)

\[u = -\frac{1}{2} - x - y, \quad v = -\frac{1}{2} + x - y, \quad w = \frac{1}{4}\]

Plug in \(u\) and solve for \(x\).
\[u = -\frac{1}{2} - x - y\]
\[0.180 = -\frac{1}{2} - x - y\]
\[0.680 = -x - y\]

Plug in \(v\) and solve for \(y\).
\[v = -\frac{1}{2} + x - y\]
\[0.220 = -\frac{1}{2} + x - y\]
\[0.720 = x - y\]
Symmetry operator 2
-Symmetry operator 4

\[
\begin{align*}
2) & \quad -x & -y & \frac{1}{2}+z \\
4) & \quad -\left(\frac{1}{2}+y \quad \frac{1}{2}-x \quad \frac{1}{4}+z\right) \\
u & = \frac{1}{2}-x-y, \quad v = -\frac{1}{2}+x-y, \quad w = \frac{1}{4}
\end{align*}
\]

Plug in u and solve for x.

\[
\begin{align*}
u & = -\frac{1}{2} -x -y \\
0.180 & = -\frac{1}{2} -x -y \\
0.680 & = -x -y
\end{align*}
\]

Subtract equations

\[
\begin{align*}
0.680 & = -x -y \\
-0.720 & = -x + y \\
-0.040 & = -2x
\end{align*}
\]

\[
0.020 = x
\]

Plug in v and solve for y.

\[
\begin{align*}
v & = -\frac{1}{2} +x -y \\
0.220 & = -\frac{1}{2} +x -y \\
0.720 & = x -y
\end{align*}
\]
Symmetry operator 2
-Symmetry operator 4

\[
\begin{align*}
2) & \quad -x \quad -y \quad \frac{1}{2} + z \\
4) & \quad -\left(\frac{1}{2} + y \quad \frac{1}{2} - x \quad \frac{1}{4} + z\right) \\
\end{align*}
\]

\[u = -\frac{1}{2} - x - y, \quad v = -\frac{1}{2} + x - y, \quad w = \frac{1}{4}\]

Plug in \(u\) and solve for \(x\).

\[
\begin{align*}
u &= -\frac{1}{2} - x - y \\
0.180 &= -\frac{1}{2} - x - y \\
0.680 &= -x - y
\end{align*}
\]

Subtract equations
\[
\begin{align*}
0.680 &= -x - y \\
-0.720 &= -x + y \\
-0.040 &= -2x
\end{align*}
\]

\[0.020 = x\]

Plug in \(v\) and solve for \(y\).

\[
\begin{align*}
v &= -\frac{1}{2} + x - y \\
0.220 &= -\frac{1}{2} + x - y \\
0.720 &= x - y
\end{align*}
\]

Add equations
\[
\begin{align*}
0.720 &= x - y \\
0.680 &= -x - y \\
1.400 &= -2y
\end{align*}
\]

\[-0.700 = y\]
How to merge atom coordinates x, y, and z from two Harker sections

| From Harker section u=1/2 we get: X₁ = -0.020 y₁ = ______ z₁ = -0.005 |
| From Harker section w=1/4 we get: X₂ = +0.020 y₂ = -0.700 z₂ = ______ |

- Note x₁ and x₂ are unequal: -0.020 ≠ +0.020.
- Both coordinate sets are correct; they describe different atoms in the unit cell (related by P4₃2₁2 symmetry) or different origin choices.
- Sadly, both coordinate sets are incomplete; y₁ and z₂ are unknown.
How to merge atom coordinates \( x, y, \) and \( z \) from two Harker sections

From Harker section \( u=\frac{1}{2} \) we get: \( X_1 = -0.020 \) \( y_1 = \ldots \) \( z_1 = -0.005 \)

From Harker section \( w=\frac{1}{4} \) we get: \( X_2 = +0.020 \) \( y_2 = -0.700 \) \( z_2 = \ldots \)

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

\[
X_1 = -0.020, \quad y_1 = \underline{y}, \quad z_1 = -0.005
\]

From Harker section $w=\frac{1}{4}$

\[
X_2 = +0.020, \quad y_2 = -0.700, \quad z_2 = \underline{y_2}
\]

Cheshire Symmetry Operators for space group $P4_{3}2_{1}2$

<table>
<thead>
<tr>
<th>1</th>
<th>X, Y, Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>-X, -Y, Z</td>
</tr>
<tr>
<td>3</td>
<td>-Y, X, 1/4+Z</td>
</tr>
<tr>
<td>4</td>
<td>Y, -X, 1/4+Z</td>
</tr>
<tr>
<td>5</td>
<td>Y, X, -Z</td>
</tr>
<tr>
<td>6</td>
<td>-Y, -X, -Z</td>
</tr>
<tr>
<td>7</td>
<td>X, -Y, 1/4-Z</td>
</tr>
<tr>
<td>8</td>
<td>-X, Y, 1/4-Z</td>
</tr>
<tr>
<td>9</td>
<td>1/2+X, 1/2+Y, Z</td>
</tr>
<tr>
<td>10</td>
<td>1/2-X, 1/2-Y, Z</td>
</tr>
<tr>
<td>11</td>
<td>1/2-Y, 1/2+X, 1/4+Z</td>
</tr>
<tr>
<td>12</td>
<td>1/2+Y, 1/2-X, 1/4+Z</td>
</tr>
<tr>
<td>13</td>
<td>1/2+Y, 1/2+X, -Z</td>
</tr>
<tr>
<td>14</td>
<td>1/2-Y, 1/2-X, -Z</td>
</tr>
<tr>
<td>15</td>
<td>1/2+X, 1/2-Y, 1/4-Z</td>
</tr>
<tr>
<td>16</td>
<td>1/2-X, 1/2+Y, 1/4-Z</td>
</tr>
<tr>
<td>17</td>
<td>X, Y, 1/2+Z</td>
</tr>
<tr>
<td>18</td>
<td>-X, -Y, 1/2+Z</td>
</tr>
<tr>
<td>19</td>
<td>-Y, X, 3/4+Z</td>
</tr>
<tr>
<td>20</td>
<td>Y, -X, 3/4+Z</td>
</tr>
<tr>
<td>21</td>
<td>Y, X, 1/2-Z</td>
</tr>
<tr>
<td>22</td>
<td>-Y, -X, 1/2-Z</td>
</tr>
<tr>
<td>23</td>
<td>X, -Y, 3/4-Z</td>
</tr>
<tr>
<td>24</td>
<td>-X, Y, 3/4-Z</td>
</tr>
<tr>
<td>25</td>
<td>1/2+X, 1/2+Y, 1/2-Z</td>
</tr>
<tr>
<td>26</td>
<td>1/2-X, 1/2-Y, 1/2-Z</td>
</tr>
<tr>
<td>27</td>
<td>1/2-Y, 1/2+X, 3/4+Z</td>
</tr>
<tr>
<td>28</td>
<td>1/2+Y, 1/2-X, 3/4+Z</td>
</tr>
<tr>
<td>29</td>
<td>1/2+Y, 1/2+X, 1/2-Z</td>
</tr>
<tr>
<td>30</td>
<td>1/2-Y, 1/2-X, 1/2-Z</td>
</tr>
<tr>
<td>31</td>
<td>1/2+X, 1/2-Y, 3/4-Z</td>
</tr>
<tr>
<td>32</td>
<td>1/2-X, 1/2+Y, 3/4-Z</td>
</tr>
</tbody>
</table>

This operator will do what we want: negate $x$
From Harker section $u=\frac{1}{2}$

$$X_1 = -0.020, \quad y_1 = \text{_______}, \quad z_1 = -0.005$$

From Harker section $w=\frac{1}{4}$

$$X_2 = +0.020, \quad y_2 = -0.700, \quad z_2 = \text{_______}$$

Apply Cheshire operator (2)

$$X_2 = -0.020, \quad y_2 = +0.700, \quad z_2 = \text{_______}$$

Cheshire Symmetry Operators for space group $P4_{3}2_{1}2$

1. $X, \quad Y, \quad Z$
2. $-X, \quad -Y, \quad Z$
3. $-Y, \quad X, \quad 1/4+Z$
4. $Y, \quad -X, \quad 1/4+Z$
5. $Y, \quad X, \quad -Z$
6. $-Y, \quad -X, \quad -Z$
7. $X, \quad -Y, \quad 1/4-Z$
8. $-X, \quad Y, \quad 1/4-Z$

This operator will do what we want: negate $x$
From Harker section $u=\frac{1}{2}$

\[ X_1 = -0.020, \quad y_1 = \_\_\_, \quad z_1 = -0.005 \]

From Harker section $w=\frac{1}{4}$

\[ X_2 = +0.020, \quad y_2 = -0.700, \quad z_2 = \_\_\_ \]

Apply Cheshire operator (2)

\[ X_2 = -0.020, \quad y_2 = +0.700, \quad z_2 = \_\_\_ \]

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 $P4_32_12$

\[
\begin{array}{cccc}
1 & X, & Y, & Z \\
2 & -X, & -Y, & Z \\
3 & -Y, & X, & 1/4+Z \\
4 & Y, & -X, & 1/4+Z \\
5 & Y, & X, & -Z \\
6 & -Y, & -X, & -Z \\
7 & X, & -Y, & 1/4-Z \\
8 & -X, & Y, & 1/4-Z \\
09 & 1/2+X, & 1/2+Y, & Z \\
10 & 1/2-X, & 1/2-Y, & Z \\
11 & 1/2-Y, & 1/2+X, & 1/4+Z \\
12 & 1/2+Y, & 1/2-X, & 1/4+Z \\
13 & 1/2+Y, & 1/2+X, & -Z \\
14 & 1/2-Y, & 1/2-X, & -Z \\
15 & 1/2+X, & 1/2-Y, & 1/4-Z \\
16 & 1/2-X, & 1/2+Y, & 1/4-Z \\
17 & X, & Y, & 1/2+Z \\
18 & -X, & -Y, & 1/2+Z \\
19 & -Y, & X, & 3/4+Z \\
20 & Y, & -X, & 3/4+Z \\
21 & Y, & X, & 1/2-Z \\
22 & -Y, & -X, & 1/2-Z \\
23 & X, & -Y, & 3/4-Z \\
24 & -X, & Y, & 3/4-Z \\
25 & 1/2+X, & 1/2+Y, & 1/2+Z \\
26 & 1/2-X, & 1/2-Y, & 1/2+Z \\
27 & 1/2-Y, & 1/2+X, & 3/4+Z \\
28 & 1/2+Y, & 1/2-X, & 3/4+Z \\
29 & 1/2+Y, & 1/2+X, & 1/2-Z \\
30 & 1/2-Y, & 1/2-X, & 1/2-Z \\
31 & 1/2+X, & 1/2-Y, & 3/4-Z \\
32 & 1/2-X, & 1/2+Y, & 3/4-Z \\
\end{array}
\]
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: \(\text{atom}_1 \rightarrow \text{atom}_2\) and \(\text{atom}_1 \leftarrow \text{atom}_2\), 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?
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 \( P4_32_12 \).
Verify your answer \( x,y,z \) is consistent with space group \( P4_32_12 \).
Which pair of symmetry-equivalent positions in space group P4321 could have produced this non-Harker peak?
Plug in \(x, y, z\) and solve for \(u, v, w\) of a non-Harker Patterson peak

Original \(x, y, z\)
\[x = -0.020, y = +0.700, z = -0.005\]

\[
\begin{align*}
symop 1 & \quad x & y & z \\
symop 5 & - (y & x & -z) \\
u = x - y & v = -x + y & w = 2z
\end{align*}
\]

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 $x, y, z$

\[ x = -0.020, \quad y = +0.700, \quad z = -0.005 \]

<table>
<thead>
<tr>
<th>symop 1</th>
<th>$x$</th>
<th>$y$</th>
<th>$z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>symop 5</td>
<td>$(y)$</td>
<td>$x$</td>
<td>$-z$</td>
</tr>
</tbody>
</table>

\[ u = x - y \quad v = -x + y \quad w = 2z \]

\[
\begin{align*}
  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
\end{align*}
\]

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

\[ u = -0.72, \quad v = 0.72, \quad w = -0.01 \]
Plug in $x, y, z$ and solve for $u, v, w$ of a non-Harker Patterson peak

**Original $x, y, z$**

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

<table>
<thead>
<tr>
<th>Symop 1</th>
<th>$x$</th>
<th>$y$</th>
<th>$z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Symop 5</td>
<td>$-y$</td>
<td>$x$</td>
<td>$-z$</td>
</tr>
</tbody>
</table>

$u = x - y, \quad v = -x + y, \quad w = 2z$

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

$u = -0.720, \quad v = 0.720, \quad w = -0.01$

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

- $u = x - y$
- $v = -x + y$
- $w = 2z$

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

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

Thus, $x = -0.02, y = 0.70, z = -0.005$ is correct.

Hurray! We are finished!
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 $\begin{array}{cccc} x & y & z \\ \end{array}$

-symop 5 $\begin{array}{cccc} y & x & -z \\ \end{array}$

$\begin{array}{cccc} u = x - y & v = -x + y & w = 2z \\ \end{array}$
An example when the $x, y, z$ does not predict $u, v, w$.

Original $x, y, z$

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

<table>
<thead>
<tr>
<th>symop 1</th>
<th>$x$</th>
<th>$y$</th>
<th>$z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>symop 5</td>
<td>$-(y)$</td>
<td>$x$</td>
<td>$-z$</td>
</tr>
</tbody>
</table>

$$u = x - y, \quad v = -x + y, \quad w = 2z$$

\begin{align*}
    u &= x - y \\
    u &= 0.020 - 0.700 \\
    u &= -0.680
\end{align*}

\begin{align*}
    v &= -x + y \\
    v &= -0.020 + 0.700 \\
    v &= 0.680
\end{align*}

\begin{align*}
    w &= 2z \\
    w &= 2(-0.005) \\
    w &= -0.010
\end{align*}

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

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

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

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

<table>
<thead>
<tr>
<th>u=x-y</th>
<th>v=-x+y</th>
<th>w=2z</th>
</tr>
</thead>
<tbody>
<tr>
<td>u=0.020-0.700</td>
<td>v=-0.020+0.700</td>
<td>w=2(-0.005)</td>
</tr>
<tr>
<td>u=-0.680</td>
<td>v=0.680</td>
<td>w=-0.010</td>
</tr>
</tbody>
</table>

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.


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.
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.
Advanced case: Proteinase K in space group $P4_{3}2_{1}2$

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

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

$P4_{3}2_{1}2$  
No. 96

$D_{4}^{8}$  
$P4_{3}2_{1}2$

422  
Tetragonal

Patterson symmetry $P4/mmm$
Advanced case, Proteinase K in space group P4_3212

- 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 P4₃2₁₂

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

1. \( x, y, z \) (reference)
2. \( x, y, \frac{1}{2} + z \)  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. \( y, x, \frac{1}{2} - z \)
8. \( y, x, \bar{z} \)
sym operator 1
-sym operator 5

\[
\begin{align*}
u &= x - y \\
v &= -x + y \\
w &= 2z
\end{align*}
\]

Original x
\[
x = -0.020, y = +0.700, z = -0.005
\]

<table>
<thead>
<tr>
<th>u=x-y</th>
<th>v=-x+y</th>
<th>w=2z</th>
</tr>
</thead>
<tbody>
<tr>
<td>u=-0.020-0.700</td>
<td>v=+0.020+0.700</td>
<td>w=2 (-0.005)</td>
</tr>
<tr>
<td>u=-0.720</td>
<td>v=+0.720</td>
<td>w=-0.010</td>
</tr>
</tbody>
</table>

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 coordinates.

Thus, \( x = -0.020, y = 0.700, z = -0.005 \) is correct.

Hurray! We are finished!

Negated x
\[
x = +0.020, y = +0.700, z = -0.005
\]

<table>
<thead>
<tr>
<th>u=x-y</th>
<th>v=-x+y</th>
<th>w=2z</th>
</tr>
</thead>
<tbody>
<tr>
<td>u=+0.020-0.700</td>
<td>v=-0.020+0.700</td>
<td>w=2 (-0.005)</td>
</tr>
<tr>
<td>u=-0.680</td>
<td>v=+0.680</td>
<td>w=-0.010</td>
</tr>
</tbody>
</table>

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 non-Harker peak.

Original x was correct.
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.

<table>
<thead>
<tr>
<th>H</th>
<th>K</th>
<th>L</th>
<th>FreeR_flag</th>
<th>SIGFP_native-jeannette</th>
<th>SIGFP_native-john</th>
<th>SIGFP_native-aj</th>
<th>SIGFP_native-joshua</th>
<th>SIGFP_native-mimi</th>
<th>SIGFP_native-wenyang</th>
<th>SIGD_eucl3-beccah</th>
<th>SIGFP_eucl3-beccah</th>
<th>D_eucl3-beccah</th>
<th>SIGD_eucl3-jessica</th>
<th>SIGFP_eucl3-jessica</th>
<th>SIGD_eucl3-jessica</th>
<th>SIGD_eucl3-jessica</th>
<th>SIGD_eucl3-jessica</th>
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</thead>
<tbody>
<tr>
<td>3</td>
<td>2</td>
<td>64</td>
<td>10.00</td>
<td>130.30</td>
<td>177.93</td>
<td>2.20</td>
<td>150.51</td>
<td>4.01</td>
<td>144.96</td>
<td>2.04</td>
<td>103.41</td>
<td>4.04</td>
<td>164.00</td>
<td>2.62</td>
<td>126.54</td>
<td>6.82</td>
<td>2.62</td>
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<tr>
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<td>2</td>
<td>65</td>
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<td>175.48</td>
<td>191.37</td>
<td>1.66</td>
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<td>3.23</td>
<td>177.46</td>
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<td>159.61</td>
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<td>202.44</td>
<td>2.22</td>
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<td>5.15</td>
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<tr>
<td>3</td>
<td>2</td>
<td>66</td>
<td>17.00</td>
<td>110.19</td>
<td>129.09</td>
<td>2.60</td>
<td>141.68</td>
<td>4.54</td>
<td>121.00</td>
<td>2.29</td>
<td>82.97</td>
<td>5.16</td>
<td>165.87</td>
<td>2.24</td>
<td>97.76</td>
<td>4.36</td>
<td>3.30</td>
</tr>
</tbody>
</table>

Etc. for thousands of reflections
Scale intensities by a constant \( (k) \) and resolution dependent exponential \( (B) \)

<table>
<thead>
<tr>
<th>H</th>
<th>K</th>
<th>L</th>
<th>intensity</th>
<th>sigma</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>10</td>
<td>106894.0</td>
<td>1698.0</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>11</td>
<td>41331.5</td>
<td>702.3</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>12</td>
<td>76203.2</td>
<td>1339.0</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>13</td>
<td>28113.5</td>
<td>513.6</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>14</td>
<td>6418.2</td>
<td>238.7</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>15</td>
<td>45946.4</td>
<td>882.7</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>16</td>
<td>26543.8</td>
<td>555.6</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>H</th>
<th>K</th>
<th>L</th>
<th>intensity</th>
<th>sigma</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>10</td>
<td>40258.7</td>
<td>1222.9</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>11</td>
<td>25033.2</td>
<td>799.8</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>12</td>
<td>24803.6</td>
<td>771.5</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>13</td>
<td>11486.3</td>
<td>423.9</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>14</td>
<td>9180.5</td>
<td>353.6</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>15</td>
<td>25038.8</td>
<td>783.0</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>16</td>
<td>21334.6</td>
<td>686.4</td>
</tr>
</tbody>
</table>

**Comparison**

\[
\frac{106894.0}{40258.7} = 2.65 \\
\frac{41331.5}{25033.2} = 1.65 \\
\frac{76203.2}{24803.6} = 3.07 \\
\frac{28113.5}{11486.3} = 2.45 \\
\frac{6418.2}{9180.5} = 0.70 \\
\frac{45946.4}{25038.8} = 1.83 \\
\frac{26543.8}{21334.6} = 1.24
\]

- Probably first crystal is larger than the second.
- Multiply Saken’s data by \( k \) and \( B \) to put the data on the same scale.
Intensity measurements were converted to structure factor amplitudes ($|F_{HKL}|$) - 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?

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

\[
P_{uvw} = \sum_{hkl} I_{hkl} \cos 2\pi(hu + kv + lw - 0)
\]
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**

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

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
Pt derivative DNA polymerase $\beta$

$P2_12_12$

1. $x, y, z$
2. $-x, -y, z$
3. $-x + 1/2, y + 1/2, -z$
4. $x + 1/2, -y + 1/2, -z$
$P4_2$
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 1\(^{st}\) Harker section. Solve for \((x,y)\) from 2\(^{nd}\) 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
  \[ O_{p1} = x, y, z \]
  \[ O_{p2} = -x, y + \frac{1}{2}, -z \]

- Space group conventions

- Projections of unit cell and symmetry.

Illustrate with asymmetric unit = Right hand
Note, in P2₁, the vector between heavy atoms always has v component = ½.

P2₁ is confined to be in the section v=½. Why?
- This plane v=½ is called a Harker section.
P2₁ 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.

\[
\begin{align*}
\mathbf{Op}_2 &= x, \ y+\frac{1}{2}, \ -z \\
-\mathbf{Op}_1 &= -(x, \ y, \ z) \\
u &= -2x, \ \frac{1}{2}, \ w = -2z \\
\mathbf{Op}_1 &= x, \ y, \ z \\
-\mathbf{Op}_2 &= -(x, \ y+\frac{1}{2}, \ -z) \\
u &= 2x, \ -\frac{1}{2}, \ w = 2z
\end{align*}
\]
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) $w=1/2$ [Wrong]

c) $v=1/2$

d) $u=1/2$
<table>
<thead>
<tr>
<th>Equation</th>
<th>Transformation</th>
<th>$u$</th>
<th>$v$</th>
<th>$w$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1) $X, Y, Z$</td>
<td>$u=2x, v=2y, w=0$</td>
<td>$0.168=2x$</td>
<td>$0.266=2y$</td>
<td>$0.075=2z$</td>
</tr>
<tr>
<td>2) $-X, -Y, Z$</td>
<td>$u=-2x, v=-2y, w=0$</td>
<td>$-0.084=x$</td>
<td>$-0.133=y$</td>
<td>$0.150=z$</td>
</tr>
<tr>
<td>3) $-x+\frac{1}{2}y+\frac{1}{2}z$</td>
<td>$u=-2x+\frac{1}{2}, v=-2y+\frac{1}{2}, w=-2z$</td>
<td>$-0.416=x$</td>
<td>$-0.133=y$</td>
<td>$0.150=z$</td>
</tr>
<tr>
<td>4) $-x+\frac{1}{2}y+\frac{1}{2}z$</td>
<td>$u=2x+\frac{1}{2}, v=2y+\frac{1}{2}, w=-2z$</td>
<td>$0.416=x$</td>
<td>$0.133=y$</td>
<td>$-0.075=z$</td>
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<td>4) $-x+\frac{1}{2}y+\frac{1}{2}z$</td>
<td>$u=2x+\frac{1}{2}, v=2y+\frac{1}{2}, w=-2z$</td>
<td>$0.416=x$</td>
<td>$0.133=y$</td>
<td>$-0.075=z$</td>
</tr>
</tbody>
</table>
4) \( \frac{1}{2}y + \frac{1}{2} - x \) \( \frac{1}{4} + z \)
5) \( -(\frac{y}{x} - x - z) \) \( u=\frac{1}{2}, \ v=\frac{1}{2} - 2x, \ w=\frac{1}{4} + 2z \)

Plug in \( v \), solve for \( x \):
\[
0.460 = \frac{1}{2} + 2x
-0.040 = 2x
0.020 = x
\]

Plug in \( w \), solve for \( z \):
\[
0.240 = \frac{1}{4} + 2z
0.010 = 2z
-0.005 = z
\]

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

Plug in \( v \), solve for \( x \):
\[
0.460 = \frac{1}{2} + 2x
-0.040 = 2x
0.020 = x
\]

Plug in \( w \), solve for \( z \):
\[
0.240 = \frac{1}{4} + 2z
0.010 = 2z
-0.005 = z
\]

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

Plug in \( v \), solve for \( y \):
\[
0.460 = -\frac{1}{2} - 2y
0.960 = -2y
-0.480 = y
\]

Plug in \( w \), solve for \( z \):
\[
0.240 = -\frac{1}{4} + 2z
0.490 = 2z
+0.245 = z
\]

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

Plug in \( v \), solve for \( y \):
\[
0.460 = -\frac{1}{2} + 2y
0.960 = 2y
+0.480 = y
\]

Plug in \( w \), solve for \( z \):
\[
0.240 = -\frac{1}{4} + 2z
0.490 = 2z
+0.245 = z
\]

-\( Y \), \( X \), \( 1/4 + Z \)
Take $u - v$, solve for $x$:

\[
\begin{align*}
u &= -\frac{1}{2} - x - y \\
-u - v &= 2x \\
(u - v)/2 &= x
\end{align*}
\]

Plug in $u$ & $v$, solve for $x$: 

\[
\begin{align*}
(0.220 - 0.180)/2 &= x \\
0.020 &= x
\end{align*}
\]

Take $u + v$ and solve for $y$:

\[
\begin{align*}
u &= -\frac{1}{2} - x - y \\
(u + v)/2 &= y
\end{align*}
\]

Plug in $u$ & $v$, solve for $y$: 

\[
\begin{align*}
(0.180 + 0.220)/2 &= y \\
0.700 &= y
\end{align*}
\]

Take $u - v$ and solve for $y$:

\[
\begin{align*}
u &= -\frac{1}{2} + x + y \\
(u - v)/2 &= y
\end{align*}
\]

Plug in $u$ & $v$, solve for $y$: 

\[
\begin{align*}
(0.180 - 0.220)/2 &= y \\
-0.020 &= y
\end{align*}
\]

Take $u + v$, solve for $x$:

\[
\begin{align*}
u &= -\frac{1}{2} + x + y \\
u + v &= 1 + 2x \\
(u + v)/2 &= x
\end{align*}
\]

Plug in $u$ & $v$, solve for $x$: 

\[
\begin{align*}
(1.400)/2 &= x \\
0.700 &= x
\end{align*}
\]

Take $u - v$, solve for $y$:

\[
\begin{align*}
u &= -\frac{1}{2} + x - y \\
(u - v)/2 &= y
\end{align*}
\]

Plug in $u$ & $v$, solve for $y$: 

\[
\begin{align*}
(0.180 - 0.220)/2 &= y \\
-0.020 &= y
\end{align*}
\]

<table>
<thead>
<tr>
<th>no</th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>xt</th>
<th>yt</th>
<th>zt</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-5</td>
<td>0.020</td>
<td></td>
<td>0.995</td>
<td>+0.020</td>
<td>0.245</td>
<td></td>
</tr>
<tr>
<td>3-6</td>
<td>0.980</td>
<td></td>
<td>0.995</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2-7</td>
<td></td>
<td>0.520</td>
<td>0.245</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>1-8</td>
<td></td>
<td>0.480</td>
<td>0.245</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2-4</td>
<td>0.020</td>
<td></td>
<td>0.300</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>1-3</td>
<td>0.980</td>
<td></td>
<td>0.700</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5-7</td>
<td></td>
<td>0.380</td>
<td>0.990</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
A list of all 32 alternative ways of assigning atomic coordinates to the Eu site

\[
\begin{array}{cccc}
 x & y & z & 0.793022 & 0.509201 & 0.002329 \\
-x & -y & z & 0.206978 & 0.490799 & 0.002329 \\
-y & x & z+1/4 & 0.490799 & 0.793022 & 0.252329 \\
y & -x & z+1/4 & 0.509201 & 0.206978 & 0.252329 \\
y & x & -z & 0.509201 & 0.793022 & 0.997671 \\
y & -x & -z & 0.490799 & 0.206978 & 0.997671 \\
x & -y & -z+1/4 & 0.793022 & 0.490799 & 0.247671 \\
x & y & -z+1/4 & 0.206978 & 0.509201 & 0.247671 \\
\end{array}
\]

(1/2, 1/2, 0)

\[
\begin{array}{cccc}
 x+1/2 & y+1/2 & z & 0.293022 & 0.009201 & 0.002329 \\
-x+1/2 & -y+1/2 & z & 0.706978 & 0.990799 & 0.002329 \\
-y+1/2 & x+1/2 & z+1/4 & 0.990799 & 0.293022 & 0.252329 \\
y+1/2 & -x+1/2 & z+1/4 & 0.009201 & 0.706978 & 0.252329 \\
y+1/2 & x+1/2 & -z & 0.009201 & 0.293022 & 0.997671 \\
y+1/2 & -x+1/2 & -z & 0.990799 & 0.706978 & 0.997671 \\
x+1/2 & -y+1/2 & -z+1/4 & 0.293022 & 0.990799 & 0.247671 \\
x+1/2 & y+1/2 & -z+1/4 & 0.706978 & 0.009201 & 0.247671 \\
\end{array}
\]

(0, 0, 1/2)

\[
\begin{array}{cccc}
 x & y & z+1/2 & 0.793022 & 0.509201 & 0.502329 \\
-x & -y & z+1/2 & 0.206978 & 0.490799 & 0.502329 \\
-y & x & z+3/4 & 0.490799 & 0.793022 & 0.752329 \\
y & -x & z+3/4 & 0.509201 & 0.206978 & 0.752329 \\
y & x & -z+1/2 & 0.509201 & 0.793022 & 0.497671 \\
y & -x & -z+1/2 & 0.490799 & 0.206978 & 0.497671 \\
x & -y & -z+3/4 & 0.793022 & 0.490799 & 0.747671 \\
x & y & -z+3/4 & 0.206978 & 0.509201 & 0.747671 \\
\end{array}
\]

(1/2,1/2,1/2)

\[
\begin{array}{cccc}
 x+1/2 & y+1/2 & z+1/2 & 0.293022 & 0.009201 & 0.502329 \\
-x+1/2 & -y+1/2 & z+1/2 & 0.706978 & 0.990799 & 0.502329 \\
-y+1/2 & x+1/2 & z+3/4 & 0.990799 & 0.293022 & 0.752329 \\
y+1/2 & -x+1/2 & z+3/4 & 0.009201 & 0.706978 & 0.752329 \\
y+1/2 & x+1/2 & -z+1/2 & 0.009201 & 0.293022 & 0.497671 \\
y+1/2 & -x+1/2 & -z+1/2 & 0.990799 & 0.706978 & 0.497671 \\
x+1/2 & -y+1/2 & -z+3/4 & 0.293022 & 0.990799 & 0.747671 \\
x+1/2 & y+1/2 & -z+3/4 & 0.706978 & 0.009201 & 0.747671 \\
\end{array}
\]
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
  \[ a=21.1 \, \text{Å} \quad b=4.8 \, \text{Å} \quad c=23.1 \, \text{Å} \]
  \[ \alpha=90.0^\circ \quad \beta=103.0^\circ \quad \gamma=90.0^\circ \]
Difference Patterson map of Zn$^{2+}$NNQQQNY

- Two strong peaks are visible in the difference Patterson map.
- The space group is P2$_1$.
- What are the coordinates of the zinc ions?

\[
\begin{align*}
\text{u} & = 0.40, \text{v} = 0.50, \text{w} = 0.42 \\
\text{u} & = 0.60, \text{v} = 0.50, \text{w} = 0.58 \\
\end{align*}
\]
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 \(u,v,w\). So, the Patterson peak coordinates tell us the relative positions of the two atoms, but not the absolute positions of the atoms.

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 \(x,y,z\).

\[
\begin{align*}
\text{Op}_2 &= -(x, y, z) \\
\text{Op}_1 &= -(x, y+\frac{1}{2}, z) \\
\end{align*}
\]

\[
\begin{align*}
u &= -2x, \quad v = \frac{1}{2}, \quad w = -2z \\
0.40 &= -2x, \quad 0.42 = -2z \\
-0.20 &= x, \quad -0.22 = z \\
\end{align*}
\]

\(P2_1\) 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.

\[
\begin{align*}
0p2 &= -x, y + \frac{1}{2}, -z \\
-0p1 &= - (x, y, z) \\
u &= -2x, \frac{1}{2}, w = -2z
\end{align*}
\]

\[
\begin{align*}
0p1 &= x, y, z \\
-0p2 &= - (-x, y + \frac{1}{2}, -z) \\
u &= 2x, -\frac{1}{2}, w = 2z
\end{align*}
\]

We could have chosen to use a different Patterson peak $(u,v,w)$
Solve for $x,z$ coordinates of Zn ion.

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**

- \(X = 0.20\), \(z = 0.70\)
- \(X = 0.80\), \(z = 0.30\)

**Choice 2**

- \(X = 0.30\), \(z = 0.30\)
- \(X = 0.70\), \(z = 0.70\)

**Choice 3**

- \(X = 0.70\), \(z = 0.20\)
- \(X = 0.30\), \(z = 0.80\)

**Choice 4**

- \(X = 0.20\), \(z = 0.20\)
- \(X = 0.80\), \(z = 0.80\)
Lesson: symmetry operators are the bridge between atomic coordinates in the crystal and Patterson peaks.

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

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

Patterson prediction $u = -2x, w = -2z$
Lesson: Check that your $x,y,z$ can predict $u,v,w$. It’s easy to make an algebraic error.

\[
\begin{align*}
(-x, y+1/2, -z) & \quad \text{Patterson prediction} \\
-(x, y, z) & \\
(-2x, 1/2, -2z) & \\
\hline
u & v & w \\
0.40 & 0.5 & 0.42 \\
0.60 & 0.5 & 0.58 \\
0.80 & 0, 0.29 \\
\end{align*}
\]

\[
\begin{align*}
u &= -2x \\
v &= -2 \cdot 0.80 = -1.6 = 0.4 \\
w &= -2z \\
w &= -2 \cdot 0.29 = -0.58 = 0.42 \\
\end{align*}
\]
**DNA polymerase β**

Pt derivative

**P2₁₂₁₂**

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, Huguette 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. This is to the fingers subdomain by a flexible polymerase sequences and implicated arrangement within structurally similar to polymerases have maintained, or possible 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 ε. It has been studied primarily in vertebrates but homologs have also been discovered in lower eukaryotes such as yeast (1) and trypanosomes (2). Although...
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+½, y+½, -z
(4) x+½, -y+½, -z

- What symmetry axes are present?
- How are the axes oriented?
How many Patterson peak are expected for a single heavy atom site in P2$_1$2$_1$2 asymmetric unit?

List the difference vectors expressions in P2$_1$2$_1$2.

Illustrate with asymmetric unit= Right hand
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 is 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. \(-x+\frac{1}{2}, y+\frac{1}{2}, -z\)
4. \(x+\frac{1}{2}, -y+\frac{1}{2}, -z\)

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 \(w=0\).