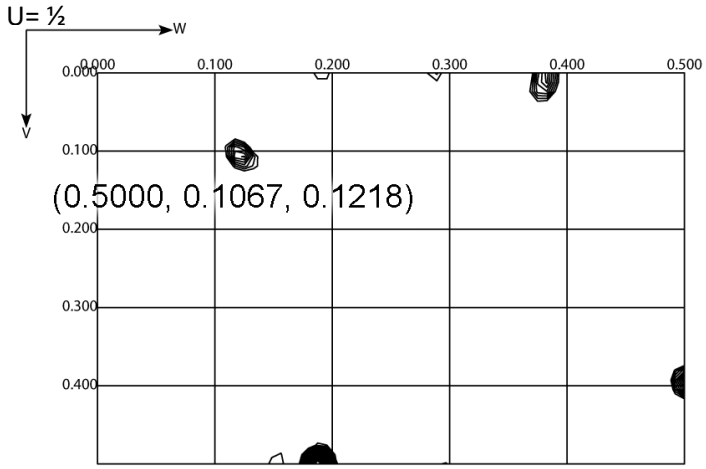

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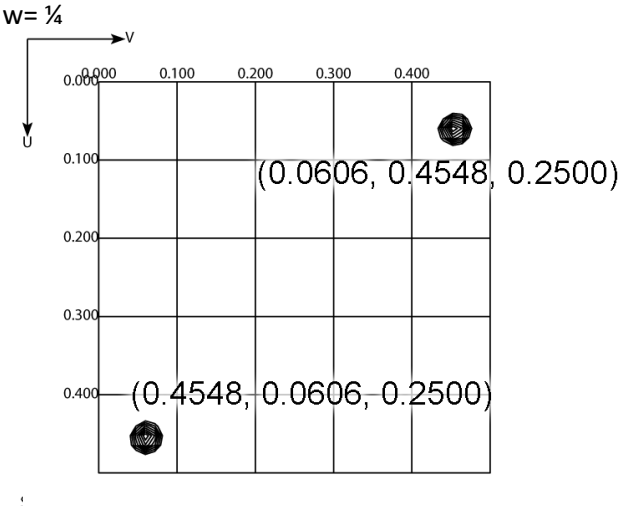
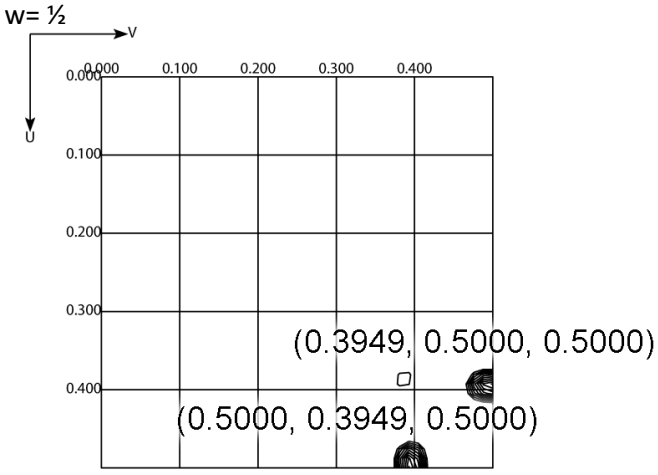
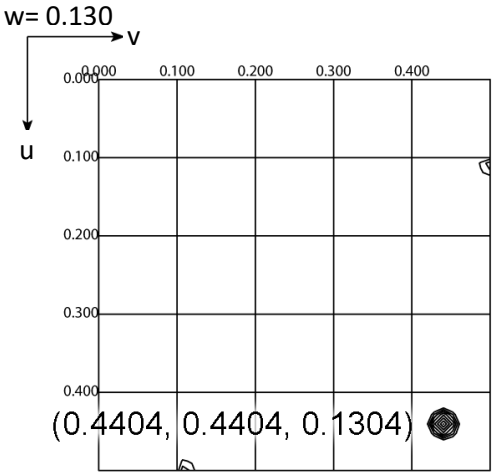
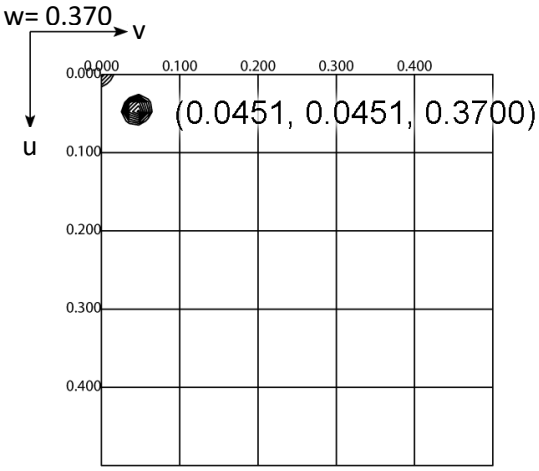
isomorphous difference Patterson map
PCMBS minus native









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Isomorphous Difference Patterson Map

ProK-PCMBS-Eric minus ProK-native-Eric

Order	No.	Site	Height/Rms	Grid			Fractional coordinates			Orthogonal coordinates		
1	1	1	149.00	0	0	0	0.0000	0.0000	0.0000	0.00	0.00	0.00
2	79	53	12.04	70	57	112	0.4888	0.3942	0.5000	33.26	26.82	50.93
3	72	47	10.30	72	2	85	0.5000	0.0110	0.3800	34.03	0.75	38.71
4	65	41	8.58	8	65	56	0.0584	0.4527	0.2497	3.97	30.81	25.43
5	64	41	8.58	65	8	56	0.4527	0.0584	0.2497	30.81	3.97	25.43
6	71	46	8.05	7	7	83	0.0469	0.0469	0.3703	3.19	3.19	37.72
7	51	33	7.19	64	64	29	0.4421	0.4421	0.1301	30.09	30.09	13.25
8	50	32	6.97	15	72	27	0.1051	0.5000	0.1203	7.15	34.03	12.26

Isomorphous Difference Patterson Worksheet. Name_____

IRS Form 1040 Date_____

1) FIRST HARKER SECTION:

a) My choice of Harker section is: u= ½

b) Enter the coordinates of the peak on this Harker section (use 3 decimal places).

u=_____0.500_____, v=_____, w=_____

c) From the table in your handout, copy your choice of difference vector appropriate for this Harker section, and the two symmetry operators used to obtain this vector.

Symmetry op. #____= _____, _____, _____

Symmetry op. #____= _____, _____, _____

Difference vector = u=_____½_____, v=_____, w=_____

1d) ↑ 1e) ↑

f) Plug in numerical values of u,v,w (1b) into equations (1d) and (1e) to solve for x or y and z. Show your work below, *neatly*.

Solve for x or y below, using equation (1d)		Solve for z below, using equation (1e)
if solving for x	if solving for y	
x=	y=	z=

2) SECOND HARKER SECTION:

a) My choice of Harker section is:__w= ¼__

b) Enter the coordinates of the peak on this Harker section (use 3 decimal places).

u=_____, v=_____, w=_____0.250_____

c) From the table in your handout, copy your choice of difference vector appropriate for this Harker section, and the two symmetry operators used to obtain this vector.

Symmetry op. #____= _____, _____, _____

Symmetry op. #____= _____, _____, _____

Difference vector = u=_____, v=_____, w=_____¼_____

2d) ↑ 2e) ↑

f) Solve for x and y. That is, plug in numerical values of u,v,w (2b) into equations (2d) and (2e). Show your work below, *neatly*.

Solve for x below, using equation (2d)	Solve for y below, using equation (2e)
x=	y=

3) CHECK CONSISTENCY BETWEEN COORDINATE SETS:

a) Coordinates from Harker #1 (step 1f): x=_____ y=_____ z=_____.

b) Coordinates from Harker #2: (step 2f) x=_____ y=_____ z=_____.

Are numerical values shared between coordinate sets in one of the dimensions? □ yes □ no.

If you answered "yes", skip the rest of this page. If you answered "no", choose one of the 32 Cheshire operators (see table in handout) that would transform coordinates (3b) to achieve one coordinate in common with (3a). List that Cheshire operator here:

_____, _____, _____.

c) Use the space below to algebraically apply the Cheshire operator to the coordinates 3b, if needed.

_____, _____, _____

_____, _____, _____

_____, _____, _____

_____, _____, _____

d) Here is my self-consistent set of heavy atom coordinates x=_____ y=_____ z=_____.

Copy these coordinates to the top of the next page.

Self-consistent set of Hg coordinates from step 3d. x=_____ y=_____ z=_____.

4) CHECK IF YOUR (X,Y,Z) CAN PREDICT THE OFF-HARKER PATTERSON PEAKS (correct hand):

Use the following difference vector equation for checking: symop. #__1__minus symop.#__5__.

Algebraic solution for the Patterson peak position:

Symmetry op. #_1_= _____x_____, _____y_____, _____z_____

Symmetry op. #_5_= _____y_____, _____x_____, _____-z_____

Difference vector= u=____x-y_____, v=___y-x_____, w=_____2z_____

a) Plug in your values of x,y,z (from 3d) , to solve for u,v,w.

u=_____, v=_____, w=_____

If your values for u,v,w are outside the range 0<u<½, 0<v<½, and 0<w<½, then apply an appropriate Patterson symmetry operator and/or add integers to fit in this range (see table in handout):

Write Patterson symop if one is needed:_____,_____,_____ .

b) (u,v,w) after applying Patterson symop: u=_____, v=_____ w=_____

Do the u,v,w on lines a or b equal (0.440, 0.440, 0.130) or (0.045, 0.045, 0.370)? □ yes □ no.

If your answer is yes: Congratulations on successfully interpreting the Patterson map! Skip to the bottom and write your final x,y,z (copy from step 3d)

If your answer is no, please negate the x value of your heavy atom coordinates, and write it here.

c) Coordinates from step 3d but with x negated. x=_____ y=_____ z=_____.

d) Plug in x,y,z values from step 4c, and re-solve for u,v,w.

u=_____, v=_____, w=_____

If your values for u,v,w are outside the range 0<u<½, 0<v<½, and 0<w<½, then apply an appropriate Patterson symmetry operator and/or add integers to fit in this range (see table in handout)

Write Patterson symop if one is needed:_____,_____,_____ .

e) (u,v,w) after applying Patterson symop: u=_____, v=_____ w=_____

Do the u,v,w values on lines d or e equal (0.440, 0.440, 0.130) or (0.045, 0.045, 0.370)? □ yes □ no.

If your answer is yes: Congratulations on successfully interpreting the Patterson map! Skip to the bottom and write your final x,y,z with "x" negated (copy from step 4c).

If your answer is no, please check your algebra from the beginning.

Write your final value of x,y,z here: x=_____y=_____z=_____.