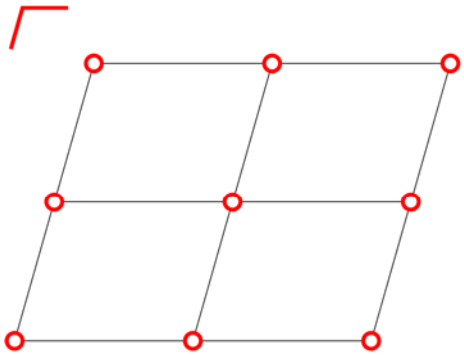
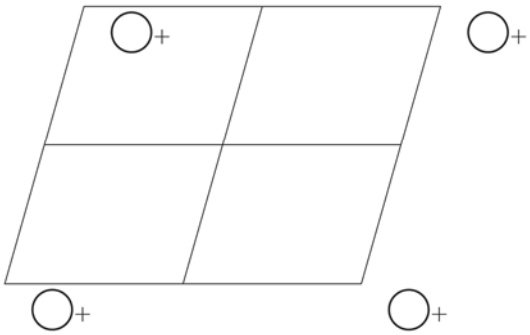
NANO 704
Final Exam

All diagrams must be carefully and legibly constructed.

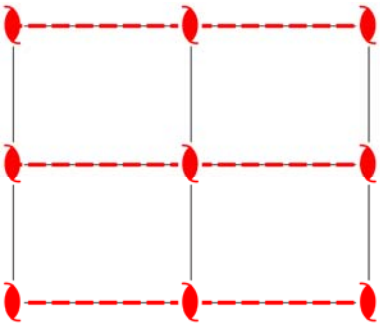
1) Graphically indicate the missing symmetry elements and complete the general-position diagrams. Show work.

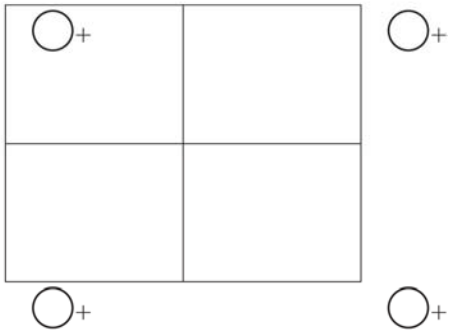
a)



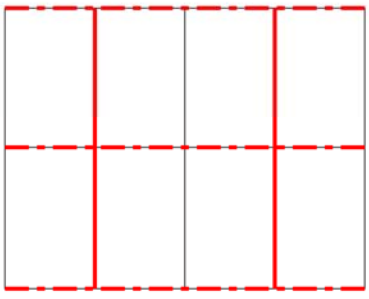


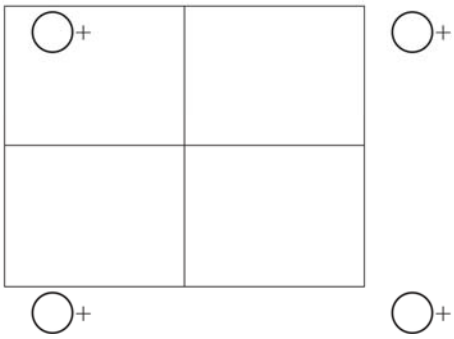
b)



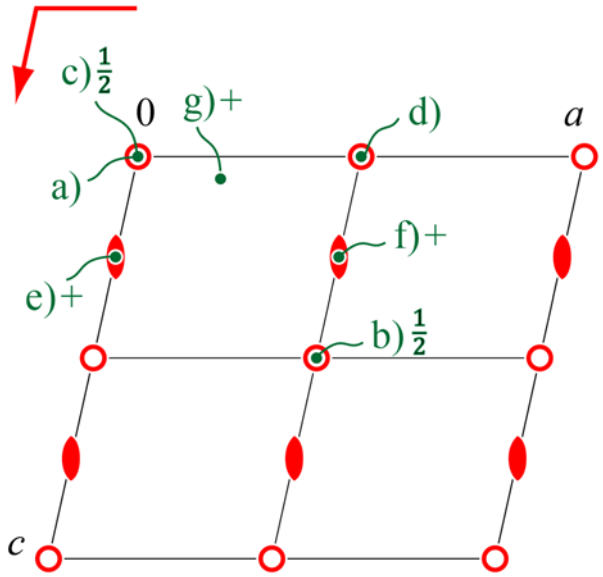


c)





2) The symmetry elements for the space group $P2/c$ are shown below.



Complete the following table:

Wyckoff letter	Multiplicity	Site Symmetry	Coordinates
g			
f			
e			
d			
c			
b			
a			

Explicit derivation of the general-position and special-position coordinates is required.

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3) For the space group $P2_1cn$:

a) Identify any reflections that have restricted phase.

b) Identify any reflections that are systematically absent.

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4) The magnitudes of the normalized structure factors E_h for the first six Fourier components from a centrosymmetric, 1-D crystal are listed below:

h	$\lvert E_h \rvert$	S_h
0	1.00	+1
1	0.70	-1
2	0.50	?
3	0.20	?
4	0.60	?
5	0.20	?

Use the Harker-Kasper inequalities to find the missing signs.

5) The electron-density $\rho(x)$ and Patterson functions $P(x)$ for 1-D crystals with point-like atoms are shown below:

The upper-left graph shows $\rho(x)$ for the AB_2 compound.

The lower-left graph shows $P(x)$ for AB_2.

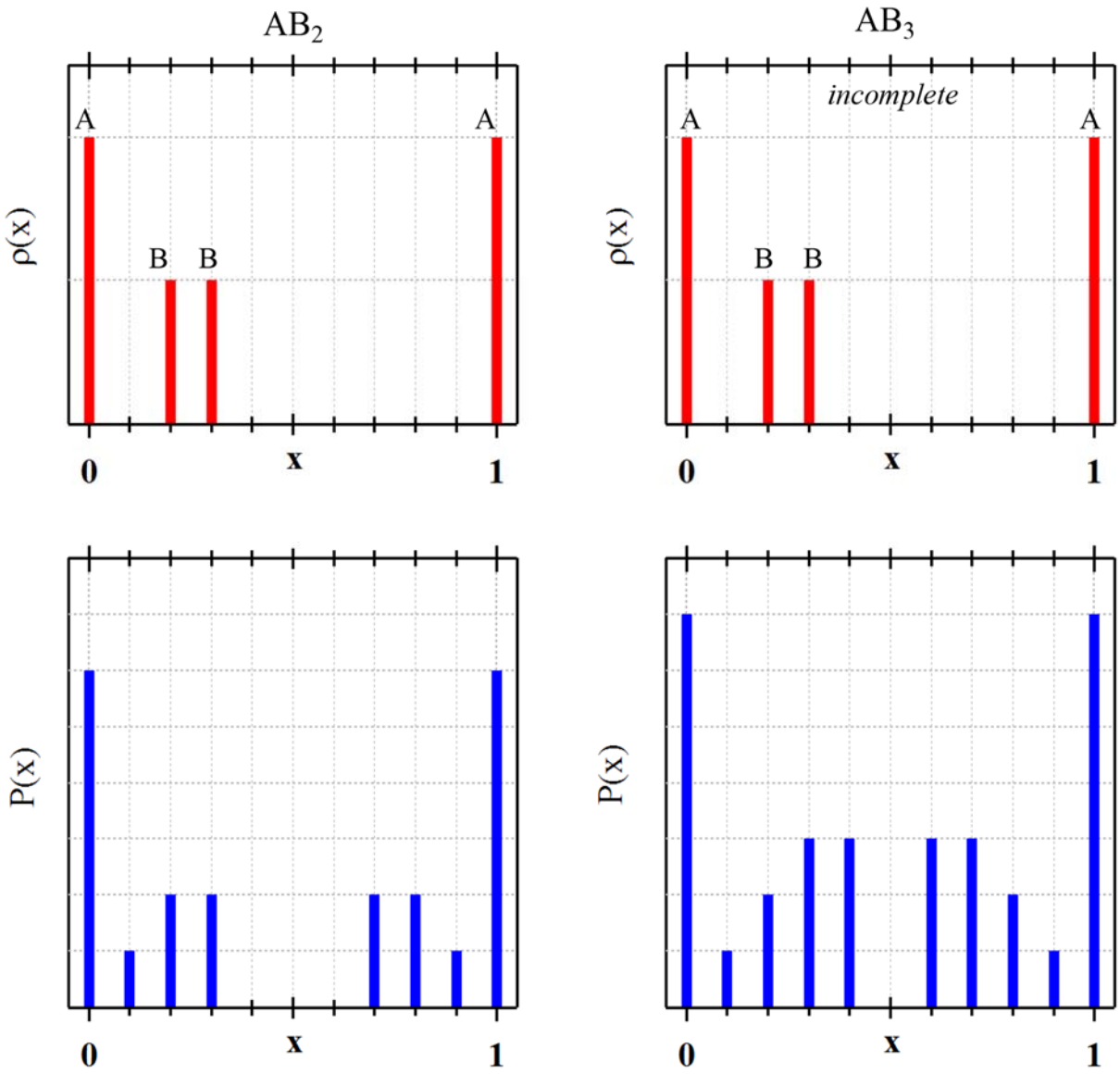
a) Label the peaks in $P(x)$ for AB_2.

An additional B atom is added to the structure to form the compound AB_3.

The lower-right graph shows $P(x)$ for AB_3.

b) Find the location of the third B atom.

c) Label all peaks in the graph of $P(x)$ for AB_3.



6) Harker lines from a pure-element crystal with space group *Pbcn* are plotted below, in terms of the coordinates (u, v, w), measured parallel to ***a***, ***b***, and ***c***, respectively.

a) Determine the general-position coordinates.

b) Determine the coordinates (x, y, z) for the general position. (Place the inversion center at the origin.)