1. What is the structure and space group (or at least, the centering, and the crystal system) of the crystal formed by alternately stacking lattices of identical atoms as in the picture below:

![Crystal Structure](image)

What are the cell parameters of the crystal in terms of the atomic radius $r$? Is there an alternate description of this structure?

2. Plot the ordered rock salt structure of the battery material LiCoO$_2$, as sections along the $c$ axis:

LiCoO$_2$: Space Group $R3m$ (166) hexagonal; $a = 2.815 \text{Å}; c = 14.072 \text{Å}.$

<table>
<thead>
<tr>
<th>Atom</th>
<th>$x$</th>
<th>$y$</th>
<th>$z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Co</td>
<td>0</td>
<td>0</td>
<td>1/2</td>
</tr>
<tr>
<td>O</td>
<td>0</td>
<td>0</td>
<td>0.238</td>
</tr>
</tbody>
</table>

*Hint:* For this space group, the $R$-centering implies addition of $(0,0,0)$, $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$ and $(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$. Any atom at $(0,0,z)$ is repeated to $(0,0,z)$.

3. The A-15 superconductors have the same structure as the following compound formed by Cr and Si:

SG = $Pm\bar{3}n$ (No. 223) $a = 4.555 \text{Å}$

<table>
<thead>
<tr>
<th>Atom</th>
<th>Wyckoff</th>
<th>$x$</th>
<th>$y$</th>
<th>$z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>2$a$</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Cr</td>
<td>6$c$</td>
<td>$1/4$</td>
<td>0</td>
<td>$1/2$</td>
</tr>
</tbody>
</table>

The space group table for SG 223 has the following:

<table>
<thead>
<tr>
<th>2$a$</th>
<th>0, 0, 0</th>
<th>$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>6$c$</td>
<td>$\frac{1}{4}, 0, \frac{1}{4}$</td>
<td>$\frac{3}{4}, 0, \frac{1}{2}$</td>
</tr>
<tr>
<td></td>
<td>$\frac{1}{2}, \frac{3}{4}, 0$</td>
<td>$0, \frac{1}{2}, \frac{1}{4}$</td>
</tr>
</tbody>
</table>

(a) What is the formula of the compound?

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1There are 12 — just plot the first four from the bottom
(b) Sketch sections of the structure for different values of \( z \).
(c) How many Cr atoms surround an Si?

4. The accompanying figure shows a two dimensional crystal structure formed by A, B, and C atoms.
   (a) What is the formula of the compound?
   (b) Identify the mirrors and rotation axes at the different atom sites.
   (c) Outline the unit cell.
   (d) What is the centering in the crystal?
   (e) Can you suggest the name of the plane group.
   (f) Provide the complete minimal crystal structure description in terms of the plane group, cell parameters and the atom positions.

5. The compound OsAl has the following structure: SG = \( Pm\bar{3}m \), \( a = 3.00 \) Å, Os at \((1/2, 1/2, 1/2)\) and Al at \((0,0,0)\).
   (a) Sketch the structure as sections, and within a cube.
   (b) What is this structure type called?
   (c) OsAl\(_2\) is formed by successively stacking OsAl cubes, but every new stack is created from the old one by adding \((1/2, 1/2, \approx 1.5)\). Sketch OsAl\(_2\) as sections after generating its coordinates. Is OsAl\(_2\) cubic? What are the cell parameters.
   (d) Can you guess the space group of OsAl\(_2\)?
   (e) Can you guess how Os\(_2\)Al\(_3\) is built up?

6. Sketch the ideal perovskite ABO\(_3\) structure with A atoms at the corners of the cell and the B atom in the middle. What are the coordinates of A, B and O? Remember to provide the minimal, crystallographic description. How many nearest neighbors do A, B, and O each have?

7. Sketch the perovskite structure as projections and then sketch the rock salt structure as projections. Compare the layers. Are there any structural relationships? Show that the perovskite structure can be considered as alternate stackings of AO rock salt layers and BO\(_2\) layers.

8. A compound is described with three kinds of atoms in the unit cell, A, B and C. A is in the Wyckoff position 2\( a \), (for the specific space group) B is in the Wyckoff position 8\( c \) and C in 24\( f \). What is the formula of the compound.

9. The electrostatic valence rule of Pauling states:

\[
\Sigma s = -V_- \quad \text{and} \quad s = V_+/Z
\]

where \( s \) is the bond valence, \( V_+ \) is the charge (valence) of the cation, \( V_- \) is the charge of the anion, and \( Z \) is the coordination number of the cation. If \( Z = 4 \) in amorphous SiO\(_2\), how many Si is each O bonded to.
(a) Assign charges on Si and O in SiO$_2$.
   Describe the Si-O network in amorphous SiO$_2$ with a sketch.
   Verify that the valence rule works for amorphous SiO$_2$.

   The addition of H$_2$O to SiO$_2$ (as happens in certain hydrothermal processes in geology) results in the Si-O-Si network of silica being broken. Use electrostatic valence to determine the H$_2$O:SiO$_2$ ratio required so that all SiO$_4$ tetrahedra are isolated, i.e. no two tetrahedra share O atoms.

(b) If Z were 6 in SiO$_2$ (giving SiO$_6$ octahedra as in stishovite SiO$_2$) how many Si would O be bonded to?

(c) TiO and TiN crystallizes in the rock-salt structure. Apply the electrostatic valence rule (you will have to chose charges). If the rule fails, attempt an explanation for why it does?