Assignment 2: The concept of space groups

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1. Diamond belongs to the $F\bar{3}dm$ with atoms in the $8a$ positions. The relevant pages for this space group taken from the international table of crystallography have been uploaded.

   a) What is the underlying crystal system?

   b) What is the underlying Bravais lattice?

   c) Draw clinographic projection showing all 8 atoms inside the unit cell. This projection can be drawn by looking down the z (or the c)-axis. Identify the 8 atoms by suitable labels and mark the fractional elevation of atoms (if $z > 0$).

   d) A four fold screw axis exists at $(\frac{1}{2}, \frac{1}{4}, 0)$. Mark its position and demonstrate the action of $\mathbf{4}_1, \mathbf{4}_2, \mathbf{4}_3$ screw operations on any atom of your choice. Clarify your working.

   e) A diamond glide plane also exists at the height $z = \frac{1}{8}$ following by the translation of $\frac{\vec{a}}{4} + \frac{\vec{b}}{4}$. Show by its action on any atom of your choice that this is indeed a symmetry operation.

   f) The m in the $Fd\bar{3}m$ space group symbol denotes a mirror plane along the face diagonal. Verify that it indeed exists in this structure.

   g) The diamond structure has a centre of inversion at $(\frac{1}{8}, \frac{1}{8}, \frac{1}{8})$. Verify this statement.

   h) A closely related structure is Zincblende (ZnS) which belongs to the space group $F\bar{4}3m$. By looking up the entry of this space group on my website, draw a clinographic projection by placing Zn at the $4a$ site and S at the $4c$ sites. Where are all the atoms located inside the unit cell?

   i) Does this zincblende structure have a center of symmetry?

2. The $P2_1/b$ (C_{2h}^5) space group is extremely well-represented in crystal structures. Its symmetry operations are shown in Figure 1.

   a) What is the crystal system and Bravais lattice type? Draw a general position at the top left of the unit cell projected onto the xy plane. What is the impact of:

   b) The $\mathbf{2}_1$ axis at $(0, \frac{1}{4}, 0)$?

   c) The centre of inversion at $(\frac{1}{2}, \frac{1}{2}, 0)$?

   d) There exists a glide plane at height $z = \frac{1}{4}$. It is parallel to the (001) plane and translates a general position by $\frac{\vec{b}}{2}$. What is the impact of this glide plane?

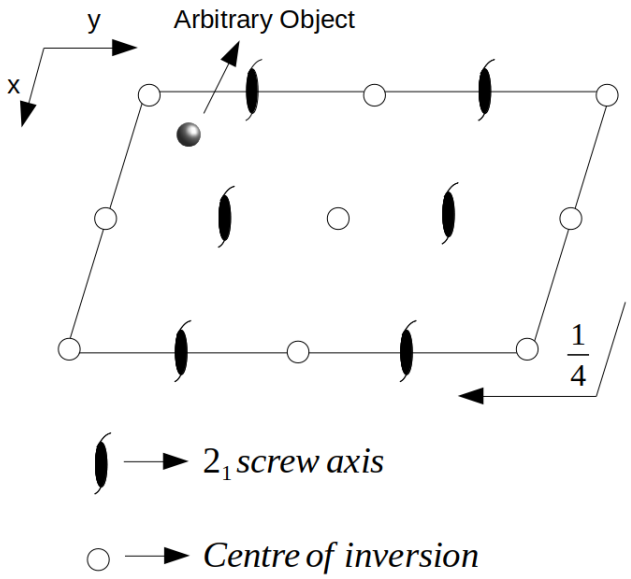

Figure 1:

3. Let's understand some nomenclature here. Consider the orthorhombic space group $Pmc2_1$. The notation tells us that the lattice type is primitive and there is:

   a) a mirror plane perpendicular to the x(or a) axis,

   b) a glide plane perpendicular to the y (or the b) axis. This means mirror planes passing through the (010) and (020) and each followed by translation $\vec{c}/2$.

   c) A $\mathbf{2}_1$ screw axis along the z (or the c) axis.
   Use a clinographic projection to find out the 4 equivalent positions in the unit cell.