1. Among others, a crystal exhibits the following planes: \((13\bar{2}), (15\bar{3}), (\bar{2}\bar{1}1), (\bar{1}2\bar{1}),\) and \((001)\)
(a) Which planes lie on a zone and what is the corresponding zone axis?
(b) Give two other planes that you would expect to lie on the same zone and show that they do.

2. Bednorz and Müller won the Nobel Prize in Physics in 1987 “for their important breakthrough in the discovery of superconductivity primarily working with Lanthanum Barium Copper Oxide.” Within that year the Paul Chu group at the University of Houston discovered that Yttrium Barium Copper Oxide (YBCO) has a \(T_c\) (superconducting transition temperature) above liquid nitrogen boiling point of 77 K. The crystal structure of YBCO belongs to space group 47 (attached at the end – page 3).

\[
\text{Y is in 1h,}
\]
\[
\text{Ba is in 2t with } z=0.1843,
\]
\[
\text{Cu_1 in 1a,}
\]
\[
\text{Cu_{II} in 2q with } z=0.3556,
\]
\[
\text{O_I in 1e,}
\]
\[
\text{O_{II} in 2s with } z=0.3779,
\]
\[
\text{O_{III} in 2r with } z=0.3790, \text{ and}
\]
\[
\text{O_{IV} in 2q with } z=0.1590.
\]

(a) Given x-ray diffraction (XRD) determined values for the spacing between the (005), (013), and (110) planes of 0.234, 0.275 and 0.273 nm, respectively, determine the a, b, and c lattice constants, which all have different values. \(\alpha=\beta=\gamma=90^\circ\).

(b) Draw the 3-D unit cell, label all atoms (write \(z\)-positions next to atoms only) and label all lattice parameters. \((\text{Make it very large as to show all the atoms and draw it roughly to scale based on your } a, b, \text{ and } c \text{ values calculated in (a)})\).

(c) What is the Bravais lattice?

(d) Calculate the theoretical density of YBCO.

(e) Based on your unit cell, how are Cu_1 and Cu_{II} coordinated with O, Y coordinated with O, and Ba coordinated with O (coordination numbers)? Make drawings of their coordinated polyhedral shapes.

(f) If you were not given the basis positions to draw your unit cell, how would you attempt to determine the coordination numbers above?

(g) Starting from the bottom and going to the top of your unit cell, what is the layer (planar) stacking sequence with chemical stoichiometries in each layer?
(h) Is the structure centric? Why?

(i) Calculate the (001) planar atomic density. Radii of Y = 0.102 nm, Ba = 0.152 nm, Cu = 0.057 nm, and O = 0.140 nm.

(j) Based on your above answers, determine the point group.

(k) The Yttrium Barium Copper Oxide (YBCO) crystal structure is a derivative of the P-cubic Perovskite crystal structure (CaTiO$_3$ is the prototype compound), determine the Perovskite structure factor (F) given Ca is at (0,0,0), Ti is at (1/2,1/2,1/2) and O is at (1/2,1/2,0), (1/2,0,1/2) and (0,1/2,1/2).

(l) For the first 12 reflections you would observe in XRD what are the values of F (leave your answers in terms of the atomic scattering factors)?

(m) Based on your answers in (l), what are the overall selection rules for the reflections observed in this compound?

(n) Calculate the XRD intensities for the (110) and (111) reflections assuming $\lambda=1.54$ Å and a=3.8 Å (consult the d-spacing Table given in class notes; Appendix 12 atomic scattering factors Table handout; Appendix 13 multiplicity factors Table handout). You may want to draw a table for your computed values. Assume CaTiO$_3$ exhibits randomly orientated grains with minimal crystal imperfection. LP = $(1+\cos^22\theta)/\sin^2\theta\cos\theta$.

(o) Even without calculating the XRD intensities as you did in (n), would you expect the (110) or the (111) reflection to have the highest XRD intensity (explain how you determined your answer)?

The following equations give the volume $V$ of the unit cell.

Cubic: $V = a^3$

Tetragonal: $V = a^2c$

Hexagonal: $V = \frac{\sqrt{3}}{2} a^2c = 0.866a^2c$

Rhombohedral: $V = a^3\sqrt{1 - 3 \cos^2 x + 2 \cos^3 x}$

Orthorhombic: $V = abc$

Monoclinic: $V = abc \sin \beta$

Triclinic: $V = abc\sqrt{1 - \cos^2 x - \cos^2 \beta - \cos^2 \gamma + 2 \cos x \cos \beta \cos \gamma}$

2
Space group 47

8 \(a\)  
\[x, y, z; \, x, y, z; \, x, y, z; \, x, y, z; \, x, y, z; \, x, y, z; \, x, y, z.\]

4 \(z\)  
\[x, y, \frac{1}{2}; \, x, y, \frac{1}{2}; \, x, y, \frac{1}{2}; \, x, y, \frac{1}{2}.\]

4 \(y\)  
\[x, y, 0; \, x, y, 0; \, x, y, 0; \, x, y, 0.\]

4 \(x\)  
\[x, \frac{1}{2}, z; \, x, \frac{1}{2}, z; \, x, \frac{1}{2}, z; \, x, \frac{1}{2}, z.\]

4 \(w\)  
\[x, 0, z; \, x, 0, z; \, x, 0, z; \, x, 0, z.\]

4 \(v\)  
\[\frac{1}{2}, y, z; \, \frac{1}{2}, y, z; \, \frac{1}{2}, y, z; \, \frac{1}{2}, y, z.\]

4 \(u\)  
\[0, y, z; \, 0, y, z; \, 0, y, z; \, 0, y, z.\]

2 \(t\)  
\[\frac{1}{2}, \frac{1}{2}, z; \, \frac{1}{2}, \frac{1}{2}, z.\]

2 \(n\)  
\[0, y, \frac{1}{2}; \, 0, y, \frac{1}{2}.\]

2 \(m\)  
\[0, y, 0; \, 0, y, 0.\]

2 \(l\)  
\[x, \frac{1}{2}, \frac{1}{2}; \, x, \frac{1}{2}, \frac{1}{2}.\]

2 \(k\)  
\[x, \frac{1}{2}, 0; \, x, \frac{1}{2}, 0.\]

2 \(j\)  
\[x, 0, \frac{1}{2}; \, x, 0, \frac{1}{2}.\]

2 \(i\)  
\[x, 0, 0; \, x, 0, 0.\]

2 \(h\)  
\[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}.\]

1 \(d\)  
\[\frac{1}{2}, 0, \frac{1}{2}.\]

1 \(c\)  
\[0, 0, \frac{1}{2}.\]

1 \(b\)  
\[\frac{1}{2}, 0, 0.\]

1 \(a\)  
\[0, 0, 0.\]