Transforming Coordinate Systems

(aka converting unit cells)

Converting from one unit cell to another related one comes up often. The process is easy and I wrote this down so I didn't have to reteach it to myself every time I needed to use it. I hope it comes in handy for others.

1. Write new basis vectors (a',b',c') in terms of old basis (a,b,c):

   $$\overrightarrow{a'} = a_1\vec{a} + a_2\vec{b} + a_3\vec{c}$$

   $$\overrightarrow{b'} = b_1\vec{a} + b_2\vec{b} + b_3\vec{c}$$

   $$\overrightarrow{c'} = c_1\vec{a} + c_2\vec{b} + c_3\vec{c}$$

   Chemically this just means draw your new unit cell axes on the old unit cell (remember right –hand rule for labeling a,b,c). Then the coordinates of the endpoint of a' in the old unit cell correspond to a_1,a_2,a_3. Ditto for b' and c'. If there is a change of origin, the coordinates of the new origin should be subtracted from the endpoint values.

2. Construct the matrix M:

   $$M = \begin{pmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{pmatrix}$$

3. Invert: $P = M^{-1}$
4. In old basis, write coordinates of new origin:

   $$T = \begin{pmatrix} o_1 \\ o_2 \\ o_3 \end{pmatrix}$$

   Chemically o_1,o_2,o_3 are just the coordinates of the new origin in the old unit cell.

5. Transform old (U) to new (U') coordinates for each atom in old unit cell:

   $$U' = P \cdot (U - T)$$

That's it! Easy as pie.