Rotate to Std Orientation
(no trig)

All math here is taken from: http://inside.mines.edu/~gmurray/ArbitraryAxisRotation/

Cell matrix, row vectors:

$$C1 = \begin{pmatrix} x1 & x2 & x3 \\ y1 & y2 & y3 \\ z1 & z2 & z3 \end{pmatrix};$$

Define the vectors for convience :

$$v1 = \begin{pmatrix} x1 \\ y1 \\ z1 \end{pmatrix};$$

$$v2 = \begin{pmatrix} x2 \\ y2 \\ z2 \end{pmatrix};$$

$$v3 = \begin{pmatrix} x3 \\ y3 \\ z3 \end{pmatrix};$$

Set up initial rotation matrix:

$$R = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix};$$

First rotate v1 about x into the xy plane:

```
length1 = Sqrt[C1[[2, 1]]^2 + C1[[3, 1]]^2]
```

$$\sqrt{y1^2 + z1^2}$$

$$R1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{y1}{length1} & \frac{z1}{length1} \\ 0 & \frac{-z1}{length1} & \frac{y1}{length1} \end{pmatrix};$$

```
R = R * R1;

C2 = Simplify[R1.C1]; C2 // MatrixForm
```

$$\begin{pmatrix} x1 & x2 & x3 \\ \sqrt{y1^2 + z1^2} & \frac{y1\, y2 + z1\, z2}{\sqrt{y1^2+z1^2}} & \frac{y1\, y3 + z1\, z3}{\sqrt{y1^2+z1^2}} \\ 0 & \frac{-y2\, z1 + y1\, z2}{\sqrt{y1^2+z1^2}} & \frac{-y3\, z1 + y1\, z3}{\sqrt{y1^2+z1^2}} \end{pmatrix}$$

Now rotate around z to get v1 parallel to the x axis:

```
projx2 = C2[[1, 1]];
```

```
projy2 = C2[[2, 1]];
```

$$\texttt{length2} = \sqrt{\texttt{projx2}^2 + \texttt{projy2}^2}\,;$$

$$\texttt{R2} = \begin{pmatrix} \frac{\texttt{projx2}}{\texttt{length2}} & \frac{\texttt{projy2}}{\texttt{length2}} & 0 \\ \frac{-\texttt{projy2}}{\texttt{length2}} & \frac{\texttt{projx2}}{\texttt{length2}} & 0 \\ 0 & 0 & 1 \end{pmatrix};$$

```
R = R * R2;
C3 = Simplify[R2.C2]; C3 // MatrixForm
```

$$\begin{pmatrix} \sqrt{x1^2 + y1^2 + z1^2} & \frac{x1\,x2 + y1\,y2 + z1\,z2}{\sqrt{x1^2 + y1^2 + z1^2}} & \frac{x1\,x3 + y1\,y3 + z1\,z3}{\sqrt{x1^2 + y1^2 + z1^2}} \\ 0 & \frac{-x2\,(y1^2 + z1^2) + x1\,(y1\,y2 + z1\,z2)}{\sqrt{y1^2 + z1^2}\,\sqrt{x1^2 + y1^2 + z1^2}} & \frac{-x3\,(y1^2 + z1^2) + x1\,(y1\,y3 + z1\,z3)}{\sqrt{y1^2 + z1^2}\,\sqrt{x1^2 + y1^2 + z1^2}} \\ 0 & \frac{-y2\,z1 + y1\,z2}{\sqrt{y1^2 + z1^2}} & \frac{-y3\,z1 + y1\,z3}{\sqrt{y1^2 + z1^2}} \end{pmatrix}$$

Now rotate about x to get v2 in the xy plane:

```
projy3 = C3[[2, 2]];

projz3 = C2[[3, 2]];
```

$$\texttt{length3} = \sqrt{\texttt{projy3}^2 + \texttt{projz3}^2}\,;$$

$$\texttt{R3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{\texttt{projy3}}{\texttt{length3}} & \frac{\texttt{projz3}}{\texttt{length3}} \\ 0 & \frac{-\texttt{projz3}}{\texttt{length3}} & \frac{\texttt{projy3}}{\texttt{length3}} \end{pmatrix};$$

C4 is the final cell matrix that has been rotated to std orientation, viz. v1 along x-axis and v2 in xy-plane, in terms of the original cell matrix:

```
R = R * R3;
C4 = FullSimplify[R3.C3]; C4 // MatrixForm
```

$$\begin{pmatrix} \sqrt{x1^2 + y1^2 + z1^2} & \frac{x1\,x2 + y1\,y2 + z1\,z2}{\sqrt{x1^2 + y1^2 + z1^2}} & \frac{x1\,x3 \ldots}{\sqrt{x\ldots}} \\ 0 & \sqrt{\frac{x2^2\,(y1^2 + z1^2) + (y2\,z1 - y1\,z2)^2 - 2\,x1\,x2\,(y1\,y2 + z1\,z2) + x1^2\,(y2^2 + z2^2)}{x1^2 + y1^2 + z1^2}} & \frac{-x1\,x3\,(y1\,y2 + z1\,z2) + (y2\,z1 - y1\,z2)\,(y3\,z1 - y1\,z3 \ldots}{(x1^2 + y1^2 + z1^2)\,\sqrt{\frac{x2^2\,(y1^2 + z1^2) + \ldots}{\ldots}}} \\ 0 & 0 & \frac{-x3\,y2\,z1 + x2\,y3\,z1 + x3\,y \ldots}{\sqrt{x1^2 + y1^2 + z1^2}\,\sqrt{\frac{x2^2\,(y1^2 + z1^2) + \ldots}{\ldots}}} \end{pmatrix}$$

C4

$$\left\{\left\{\sqrt{x1^2+y1^2+z1^2},\ \frac{x1\,x2+y1\,y2+z1\,z2}{\sqrt{x1^2+y1^2+z1^2}},\ \frac{x1\,x3+y1\,y3+z1\,z3}{\sqrt{x1^2+y1^2+z1^2}}\right\},\right.$$

$$\left\{0,\ \sqrt{\frac{x2^2\left(y1^2+z1^2\right)+(y2\,z1-y1\,z2)^2-2\,x1\,x2\,(y1\,y2+z1\,z2)+x1^2\left(y2^2+z2^2\right)}{x1^2+y1^2+z1^2}},\right.$$

$$\left(-x1\,x3\,(y1\,y2+z1\,z2)+(y2\,z1-y1\,z2)\,(y3\,z1-y1\,z3)+x1^2\,(y2\,y3+z2\,z3)+x2\left(x3\left(y1^2+z1^2\right)-x1\,(y1\,y3+z1\,z3)\right)\right)\Big/$$

$$\left.\left(\left(x1^2+y1^2+z1^2\right)\sqrt{\frac{x2^2\left(y1^2+z1^2\right)+(y2\,z1-y1\,z2)^2-2\,x1\,x2\,(y1\,y2+z1\,z2)+x1^2\left(y2^2+z2^2\right)}{x1^2+y1^2+z1^2}}\right)\right\},$$

$$\left.\left\{0,\ 0,\ \frac{-x3\,y2\,z1+x2\,y3\,z1+x3\,y1\,z2-x1\,y3\,z2-x2\,y1\,z3+x1\,y2\,z3}{\sqrt{x1^2+y1^2+z1^2}\ \sqrt{\frac{x2^2\left(y1^2+z1^2\right)+(y2\,z1-y1\,z2)^2-2\,x1\,x2\,(y1\,y2+z1\,z2)+x1^2\left(y2^2+z2^2\right)}{x1^2+y1^2+z1^2}}}\right\}\right\}$$