Allright. There's some code here, and it does stuff.

```
rrEchelon.py  Takes a matrix and returns its reduced row echelon form.
getSyms.py    Uses a couple of generators to find the 48 symmetries of a
                cubic crystal. It dumps them out to S.pkl.
S.pkl         List of numpy matrices, each one corresponding to a point
                group symmetry of a cubic crystal
fcc?NN.py     Little code that spits out the constraints on the components
                of the ?NN force constant tensor for an FCC crystal.
fcc.py        Spits out constraints for 1-8NN.  Add more NN by adding
                their one of their vectors to the list, V.

mat2vec.py    This is the interesting one.
```

Some pair of atoms in a crystal is 'connected' by some vector. The connection is made mathematically with a force constant tensor. We'll talk 3D from here on out. Without knowing any better, we write:

$$F = \begin{pmatrix} F_{11} & F_{12} & F_{13} \\ F_{12} & F_{22} & F_{23} \\ F_{13} & F_{32} & F_{33} \end{pmatrix} \tag{1}$$

And you can see that we have 9 degrees of freedom (DOF). It seems likely that some of the magical symmetries of the crystal will reduce the DOF. We can look into this by taking one of the 3×3 representations of the point group symmetries, S_s, and applying it to the F, requiring that F remain unchanged. That looks like so:

$$S_s = \begin{pmatrix} S^s_{11} & S^s_{12} & S^s_{13} \\ S^s_{21} & S^s_{22} & S^s_{23} \\ S^s_{31} & S^s_{32} & S^s_{33} \end{pmatrix} \tag{2}$$

$$S_s^{\mathrm{T}} F S_s = F \tag{3}$$

That equation, is rather intimidating, so we rewrite it thusly:

$$S_s^{\mathrm{T}} F - F S_s^{-1} = 0 \tag{4}$$

This looks a lot like the oh so familiar Lyapunov Equation:

$$AX + XB = C \tag{5}$$

where A, B, C and X are all square matrices of dimension N. So let us consider it. It is clear that all the terms on the left-hand side of the equation are linear in the components of X, thus, their sum must be linear in the components of X. This means that we may rewrite the equation as follows:

$$Mx + b = 0 \tag{6}$$

where M is a $N^2 \times N^2$ matrix, and y and b are N^2-vectors. The order in which you choose to map the components of the matrix X into the vector x is arbitrary; however, once you choose an order, you must be consistent. Let's just show one example... you could write:

$$x = \begin{pmatrix} x_{11} \\ x_{12} \\ x_{13} \\ x_{21} \\ x_{22} \\ x_{23} \\ x_{31} \\ x_{32} \\ x_{33} \end{pmatrix} \tag{7}$$

Which would imply the same ordering for b, where the components would be given by $-C_{ij}$.

Let's construct the matrix $Z \equiv AX + XB$. For the 3x3 case, we have:

$$Z = \begin{pmatrix} A_{11}X_{11} + A_{12}X_{21} + A_{13}X_{31} & A_{11}X_{12} + A_{12}X_{22} + A_{13}X_{32} & A_{11}X_{13} + A_{12}X_{23} + A_{13}X_{33} \\ A_{21}X_{11} + A_{22}X_{21} + A_{23}X_{31} & A_{21}X_{12} + A_{22}X_{22} + A_{23}X_{32} & A_{21}X_{13} + A_{22}X_{23} + A_{23}X_{33} \\ A_{31}X_{11} + A_{32}X_{21} + A_{33}X_{31} & A_{31}X_{12} + A_{32}X_{22} + A_{33}X_{32} & A_{31}X_{13} + A_{32}X_{23} + A_{33}X_{33} \end{pmatrix} + \begin{pmatrix} X_{11}B_{11} + X_{12}B_{21} + X_{13}B_{31} & X_{11}B_{12} + X_{12}B_{22} + X_{13}B_{32} & X_{11}B_{13} + X_{12}B_{23} + X_{13}B_{33} \\ X_{21}B_{11} + X_{22}B_{21} + X_{23}B_{31} & X_{21}B_{12} + X_{22}B_{22} + X_{23}B_{32} & X_{21}B_{13} + X_{22}B_{23} + X_{23}B_{33} \\ X_{31}B_{11} + X_{32}B_{21} + X_{33}B_{31} & X_{31}B_{12} + X_{32}B_{22} + X_{33}B_{32} & X_{31}B_{13} + X_{32}B_{23} + X_{33}B_{33} \end{pmatrix} \tag{8}$$

We see that Z_{12} depends on the 1$^{\text{st}}$ row of A, the 2$^{\text{nd}}$ column of X, the 1$^{\text{st}}$ row of X, and the 2$^{\text{nd}}$ column of B. More generally:

$$Z_{ij} = \sum_k A_{ik}X_{kj} + B_{kj}X_{ik} \tag{9}$$

Because of our choice of mapping from X to x, the Z_{ij} tells you what row in M you are dealing with. The indices on the variables X_{kj} or X_{ik} tell you which column in M. All that is left is to add the A_{ik} and B_{kj} into the slots in M, so given. This is difficult to show explitily, howevere, this is the best I got:

$$M = \begin{pmatrix} M_{11} & M_{12} & \dots & M_{19} \\ M_{21} & M_{22} & \dots & M_{29} \\ \vdots & \vdots & \ddots & \vdots \\ M_{91} & M_{92} & \dots & M_{99} \end{pmatrix} \leftarrow \begin{pmatrix} \{Z_{11}, X_{11}\} & \{Z_{11}, X_{12}\} & \dots & \{Z_{11}, X_{33}\} \\ \{Z_{21}, X_{11}\} & \{Z_{21}, X_{12}\} & \dots & \{Z_{21}, X_{33}\} \\ \vdots & \vdots & \ddots & \vdots \\ \{Z_{33}, X_{11}\} & \{Z_{33}, X_{12}\} & \dots & \{Z_{33}, X_{33}\} \end{pmatrix} \tag{10}$$

The left and center of the equation are M and the components of M. The thing on the right is supposed to indicate that any time you have Z_{ij} on the left in Eq. 9, and an X_{mn} next to one of the coefficients A_{pq} or B_{rt} on the right, you add that coefficient at the slot marked $\{Z_{ij}X_{mn}\}$ in M. The problem $AX + XB = C$ has now been reduced to $Mx + b = 0$, which linear algebra tells us how to solve.

For our particular case, we wish to find the constraints on the components of F. Simply take $A \to S_s^{\mathrm{T}}$, $B \to S_s^{-1}$, $X \to F$ in Eq. 5, and $C = 0$ and then put M into reduced row echelon form. Reading off the rows gives you the constraints on the components of F. For exmpample, you may end up with somthing that looks like this:

```
 xx  xy  xz  yx  yy  yz  zx  zy  zz
[ 0.  1.  0.  0.  0.  0.  0.  0.  0.]
[ 0.  0.  1.  0.  0.  0.  0.  0.  0.]
[ 0.  0.  0.  1.  0.  0.  0.  0.  0.]
[ 0.  0.  0.  0.  1.  0.  0.  0. -1.]
[ 0.  0.  0.  0.  0.  1.  0.  0.  0.]
[ 0.  0.  0.  0.  0.  0.  1.  0.  0.]
[ 0.  0.  0.  0.  0.  0.  0.  1.  0.]
```

Which we can rewrite like so:

```
xy                          = 0
    xz                      = 0
        yx                  = 0
            yy          -zz = 0
                yz          = 0
                    zx      = 0
                        zy  = 0
```

We see, then, that there are two DOF. Both $yy = zz$, and xx may be varied independently This particular force constant tensor is axially symmetric.

If there are n symmetry elements, S_s, that can transform your bond vector back onto itself, you simply stack up the n M_s, and find the reduced row echelon form of M:

$$M = \begin{pmatrix} M_1 \\ M_2 \\ \vdots \\ M_n \end{pmatrix} \tag{11}$$