The following is how NITROGEN calculates the NC_TRANS matrix and how CFOUR can be used to generate the same.

First, we need the F matirx (Hessian). CFOUR's units are in Bohr while NITROGEN uses Angstrom. Therefore, every internal coordinate from FCMINT needs to be scaled accordingly. Angles should remain untouched, so each row with a radius needs to be converted as well as each column with a radius. I am unsure why, but for the water molecule, row three and column three need to be converted to angstroms in the G matrix.

$L^{-1}GFL = \Lambda$

L and Λ are column swapped so that the eigenvalues are sorted in ascending order. Then comes a weird chunk of code I found in surf.c (NITROGEN) that scales L so that $L^{-1}FL$ yields the diagonalized F with frequencies along the diagonal. See 'NITROGEN' for those notes. Then L^{-1T} yields the left block of NC_TRANS. The right most column is $L^{-1}q$ Where q is the IC eq. geometry.