Problem 1 (Rotation Matrices). Define $SO(3)$ to be the set of all rotation matrices $R$, i.e. $3 \times 3$ real matrices such that $R^T R = I$ ($I$ denotes the $3 \times 3$ identity matrix) and $\det R = 1$. Show that there exists a pair $(e^{i\theta}u, u)$ uniquely determined up to reflection $(e^{-i\theta}, -u)$, where $\theta$ is real and $u \in \mathbb{R}^3$ is a unit vector, such that for all $x \in \mathbb{R}^3$ we have

$$Rx = u(u \cdot x) + [x - u(u \cdot x)]\cos \theta + (u \times x)\sin \theta.$$ 

Problem 2 (Quaternions for rotations). Define the complex matrices

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$ 

If $x = (x_1, x_2, x_3) \in \mathbb{R}^3$ then define $X(x) = \sigma_1 x_1 + \sigma_2 x_2 + \sigma_3 x_3$. If $u = (u_1, u_2, u_3) \in \mathbb{R}^3$ is a unit vector and $\theta$ is a real number, define $H(e^{i\theta}, u) = \sigma_0 \cos(\theta/2) - i(\sigma_1 u_1 + \sigma_2 u_2 + \sigma_3 u_3) \sin(\theta/2)$. If $H$ is a $2 \times 2$ complex matrix let $H^H$ denote its complex conjugate transpose. Suppose $R$ is a rotation matrix as in problem 1 above. Then show that $X(Rx) = H(e^{i\theta}, u)X(x)H(e^{i\theta}, u)^H$, where $(e^{i\theta}, u)$ correspond to $R$ as in problem 1.

Problem 3 (Internal coordinates via coordinate transformations). Define the following matrices:

$$T_0(l) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ l & 0 & 0 & -1 \end{pmatrix}, \quad T_1(c) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -c & 0 & s \\ 0 & 0 & -1 & 0 \\ 0 & s & 0 & c \end{pmatrix}, \quad T_2(z) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & x & -y & 0 \\ 0 & y & x & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

where $l > 0$, $-1 < c < 1$, $s = \sqrt{1 - c^2}$, $z = x + iy$, and $x^2 + y^2 = 1$. If $\mathcal{X}(A) \in \mathbb{R}^3$ denotes the position of atom $A$ recall we defined the conformed pose, pose($A, b, t$), where $A$ is an atom contained in the bond $b$, which is in turn contained in the triangle $t$, by the rule:

$$\text{pose}(A, b, t) = (e_0, e_1, e_2, e_3), \quad e_0 = \mathcal{X}(A),$$

$$e_3 = \frac{\mathcal{X}(A') - \mathcal{X}(A)}{||\mathcal{X}(A') - \mathcal{X}(A)||}, \quad e_1 = \frac{\mathcal{X}(A'') - \mathcal{X}(A) - e_3 \{ e_3 \cdot [\mathcal{X}(A'') - \mathcal{X}(A)] \}}{||\mathcal{X}(A'') - \mathcal{X}(A) - e_3 \{ e_3 \cdot [\mathcal{X}(A'') - \mathcal{X}(A)] \}||},$$

$$e_2 = e_3 \times e_1,$$

where $b = \{A, A'\}$ and $t = \{A, A', A''\}$. These formulae make sense provided the triangle $t$ is noncollinear in the configuration $\mathcal{X}$. Verify the following assertions.

1. If the bond $b$ has length $l$ then pose($A', b, t$) = pose($A, b, t$)T_0(l).
2. If an angle $a = \{b_1, b_2\}$ has the common atom $A$, and bond angle cosine $c = \cos \theta$, then pose($A, b', t(a)$) = pose($A, b, t(a)$)T_1(c).
3. If a wedge $w = \{t_1, t_2\}$ has the common bond $b = \{A, A'\}$, and the wedge angle coordinate is $z = e^{i\theta}$ relative to the orientation $[A_{1j}'; A, A', A_{2j}]$, where $A_{1j} \in t_j \setminus b$, $j = 1, 2$, then pose($A, b, t_2$) = pose($A, b, t_1$)T_2(e^{i\theta}).