MATH 728A, BIOMOLECULAR GEOMETRY, HOMEWORK #8

Problem 1 (Identities). Prove the following identities involving the matrices defined in homework 7.3. $T_0(l)^{-1} = T_0(l), T_1(c)^{-1} = T_1(c), T_2(z)^{-1} = T_2(\bar{z})$, and $T_2(z)T_0(l) = T_0(l)T_2(\bar{z})$.

Problem 2 (Spherical coordinates via coordinate transformations). Consider a wedge $w = \{t, t'\}$, where $t = \{A, A', A''\}$, $t' = \{A', A'', A'''\}$, $b = \{A, A'\}$, and $b' = \{A', A''\}$. Show that $\text{pose}(A, b, t)T_0(l)T_1(c)T_2(z) = \text{pose}(A', b', t')$, where l is the bond length of b, $c = \cos(\theta)$ and θ is the bond angle of $\{b, b'\}$, and $z = e^{i\phi}$ where ϕ is the wedge angle for the wedge w with respect to the orientation $[A, A', A'', A''']$. Use this relation to compute the coordinates of the atom A in $\text{pose}(A', b', t')$. Explain the relation of this with spherical coordinates.

Problem 3 (Spherical Trigonometry: Law of Cosines). Use the notation of problem 2. Let $c' = \cos\theta'$, where θ' is the bond angle for $\{\{A', A''\}, \{A', A'''\}\}$. Use the notation $\text{pose}(A, b, t) = \text{pose}(A, A', A'')$, since the 3-tuples (A, b, t) and (A, A', A'') contain exactly the same information. Show that $\text{pose}(A', A, A'')T_1(c)T_2(z)T_1(c') = \text{pose}(A', A''', A'')$. Let τ denote the bond angle of $\{\{A, A'\}, \{A', A'''\}\}$. Note that $\cos\tau$ is the dot product of the $\mathbf{e}_3$ vector of $\text{pose}(A', A, A'')$ with the $\mathbf{e}_3$ vector of $\text{pose}(A', A''', A'')$. Using the matrix product $T_1(c)T_2(z)T_1(c')$ verify the *law of cosines* from spherical trigonometry: $\cos\tau = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos\phi$.

Problem 4 (Spherical Trigonometry: Law of Sines). Use the notation of problems 2 and 3. Compute the spherical coordinates of the point $\mathcal{X}(A)$ in the $\text{pose}(A', A''', A'')$. Verify the *law of sines* from spherical trigonometry: $\frac{\sin\psi}{\sin\theta} = \frac{\sin\phi}{\sin\tau}$, where $\text{pose}(A', A''', A) = \text{pose}(A', A''', A'')T_2(e^{i\psi})$. Show that ψ is the wedge angle for $\{\{A', A'', A'''\}, \{A, A', A'''\}\}$ with respect to the same orientation as in problem 2.

Problem 5 (Tetrahedronometry). Use the notation of problem 2. Compute the rectangular and spherical coordinates of the point $\mathcal{X}(A)$ in the $\text{pose}(A''', A'', A')$ in terms of the bond lengths of $b = \{A, A'\}, b' = \{A', A''\}, b'' = \{A'', A'''\}$, and the bond angles of $\{b, b'\}$ and $\{b', b''\}$.