

CORRECTIONS AND CLARIFICATIONS

Homework 1, Problem 1. In Part (3) one should insert the words *labelled with* between the phrase *and the edges are* and the phrase *(oriented) wedge angles*. Part (4) needs to be done before the signs of the numerical labels of the wedges in Part (3) can be determined. Or you might use the formulae that I gave in class to compute the improper dihedral angle ϕ (for some choice of the orientations of those improper) but then you should choose the orientations of the tetrahedra in Part (4) to match the orientations of the improper. So if $d = (a_1, a_2)$ is an oriented improper where $a_1 = \{\{A_1, A_2\}, \{A_2, A_3\}\}$ and $a_2 = \{\{A_4, A_2\}, \{A_2, A_3\}\}$ then a consistent choice of the orientation of the corresponding tetrahedron $\{A_1, A_2, A_3, A_4\}$ is the equivalence class of (A_1, A_2, A_3, A_4) .

After you create the molecule in IMIMOL and before you export the MOPAC Z-matrix for the molecule, you should change all the bond lengths to 1.0. If you leave the bond lengths as $\sqrt{3} = 1.732$ you will not see anything when you try to display the molecule in RASMOL. If in RASMOL you choose the menu option Display/BallandStick you will see the atoms but no bonds. This is because RASMOL knows too much chemistry; a carbon atom and a hydrogen atom that are 1.732 angstroms (1 angstrom is 10^{-10} meter) apart will not be chemically bonded, so RASMOL will not draw a line between them. A typical *CH* bond length is about 1 angstrom.

Homework 1, Problem 2. I neglected to tell you which pairs of atoms are bonded. They are: $C_1H_1, C_1H_2, C_1H_3, C_2H_4, C_2H_5, C_2H_6, C_1C_2$.

You will need at least one torsion angle in your triangle/wedge tree. Let us suppose that this torsion is $\{a_1, a_4\}$, where $a_1 = \{\{H_1, C_1\}, \{C_1, C_2\}\}$ and $a_4 = \{\{C_1, C_2\}, \{C_2, H_4\}\}$. The corresponding wedge is $\{\{H_1, C_1, C_2\}, \{C_1, C_2, H_4\}\}$, and the tetrahedron of this wedge is $\{H_1, C_1, C_2, H_4\}$. We have stated that one does not need to orient a torsion in order for its numerical label to be geometrically meaningful. This is because the equivalence class of (H_1, C_1, C_2, H_4) is the same as that of (H_4, C_2, C_1, H_1) . Thus there is a canonical orientation of the tetrahedron associated to any torsion. However, it is possible to choose the orientation of this tetrahedron opposite to the canonical one shown above; e.g. the equivalence class of (C_1, H_1, C_2, H_4) . If you choose to do that then you should label the wedge with the negative of the torsion angle.

Homework 2, Problem 2. When you print out a stereo picture, you must include labels in your picture. Otherwise the point of the problem is lost.

Homework 2, Problem 3. When you print out stereo pictures, you should include labels in your pictures, and indicate on each picture the value of the torsion angle corresponding to that picture.

Homework 7, Problem 2. We should use the notation $H(e^{i\theta}, \mathbf{u}) = \sigma_0 \cos \theta - iX(\mathbf{u}) \sin \theta$ instead of what is given in the problem statement: $H(e^{i\theta}, \mathbf{u}) = \sigma_0 \cos(\theta/2) - iX(\mathbf{u}) \sin(\theta)$. This is because $e^{i\theta} = e^{i(\theta+2\pi)}$, and yet $\cos(\theta/2) = -\cos((\theta+2\pi)/2)$ and $\sin(\theta/2) = -\sin((\theta+2\pi)/2)$. With the new and now correct definition of $H(e^{i\theta}, \mathbf{u})$ the problem is

to prove the relation: $H(e^{i\theta/2}, \mathbf{u})X(\mathbf{x})H(e^{i\theta/2}, \mathbf{u})^\dagger = X(R\mathbf{x})$ when R rotates by θ around the axis \mathbf{u} . Thus both of the 2×2 matrices $H(e^{i\theta/2}, \mathbf{u})$ and $H(-e^{i\theta/2}, \mathbf{u}) = -H(e^{i\theta/2}, \mathbf{u})$ represent the same rotation matrix R . Thus there are two “quaternions” for every rotation.