MATH 728A, BIOMOLECULAR GEOMETRY, HOMEWORK #1

Problem 1 (Methane). Consider an idealized molecule of methane CH_4 where the positions of the atoms are $C(1,1,1), H_1(0,0,0), H_2(2,2,0), H_3(2,0,2), H_4(0,2,2)$. Each of the hydrogen atoms is bonded to the carbon atom. Show that the four hydrogens are at the vertices of a regular tetrahedron, and the carbon is at its center. Compute the following.

(1) The atom/bond tree $\Gamma^{(0)}$, where the edges are labelled with bond lengths.
(2) A bond/angle tree $\Gamma^{(1)}$, where the vertices are the edges of $\Gamma^{(0)}$ and the edges (angles) are labelled with bond angles.
(3) A triangle/wedge tree $\Gamma^{(2)}$, where the vertices are triangles corresponding to the edges of $\Gamma^{(1)}$ and the edges are (oriented) wedge angles.
(4) For each edge in $\Gamma^{(2)}$, give the corresponding 3-simplex, and give the chosen orientation of that 3-simplex to match the assigned wedge angle.

Use this information to create this molecule in IMIMOL; export a MOPAC Z-matrix and a RASMOL label file, and visualize the molecule using RASMOL.

Problem 2 (Ethane). Consider an idealized molecule of ethane where the positions of the atoms are $C_1(1,1,1), C_2(0,0,0), H_1(2,2,0), H_2(2,0,2), H_3(0,2,2), H_4(-1,-1,1), H_5(1,-1,-1), H_6(-1,1,-1)$. Compute the same four items as in Problem #1. Create this molecule in IMIMOL but change the CC bond length to 1.54 and all the CH bond lengths to 1.1. Draw the molecule using RASMOL.

Problem 3 (Stereo Viewing). Use cross-eyed stereo to look at the enclosed picture of cyclohexane. Rank order (approximately) the 18 atoms from closest to the viewer to farthest from the viewer.