1010-53-78 **Daniel B. Dix*** (dix@math.sc.edu), 400E LeConte, Department of Mathematics, University of South Carolina, Columbia, SC 29208. *Graphs for indexing coordinates specifying molecular shape in 3D space and some applications.*

An *unoriented Z-system* is a triple (τ_1, τ_2, τ_3) where τ_1 is a tree graph, τ_2 is a spanning tree in the line graph of τ_1 and τ_3 is a spanning tree in the line graph of τ_2. Let each vertex of τ_1 represent an atom in a molecule, and let each edge of τ_1 be labeled with the distance in 3D space between the two atoms involved. Let each edge α of τ_2 be labeled with an angle $0 < \theta < \pi$, thought of as the angle in space between the two line segments determined by the two vertices of α. Let each edge ω of τ_3 be labeled with a pair (w^*, φ), where $-\pi < \varphi \leq \pi$ is a signed angle between the two half-planes of the two space triangles associated to the two vertices of ω. The half-planes meet in the line containing the line segment common to the two triangles. w^* is a combinatorial object designed to distinguish between the tetrahedron determined by the four atoms involved in ω and its mirror image. Theorem: this data uniquely determines the shape of the molecule. We use this formalism to parameterize the geometry of molecular hexagons. Z-systems for biological polymers can be obtained by gluing together the Z-systems of small monomer molecules. (Received August 19, 2005)