CY40014 Introduction to Computational Chemistry
Autumn 2010-2011

Worksheet 8

Module 3: Introduction to Molecular Modelling

Aim of the present module

1. To obtain standard molecular parameters such as bond length, bond angle and dihedral angle starting from geometric representation of molecules.
2. The Z-matrix
3. Simple quantum chemical calculations using standard softwares.

Molecular geometry

We are going to obtain some essential information regarding a molecule using the concept of vector algebra.

W8_1. Given two vectors: $\vec{v}_1:(x_1\ y_1\ z_1)$ and $\vec{v}_2:(x_2\ y_2\ z_2)$. Find the vector $\vec{v}_{21}=\vec{v}_2-\vec{v}_1$. What is the physical significance of the vector $\vec{v}_{21}$?

W8_2. Given three points: $P:(x_1\ y_1\ z_1)$, $Q:(x_2\ y_2\ z_2)$ and $R:(x_3\ y_3\ z_3)$. Obtain the angle PQR. Report the value both in degrees and radians.

W8_3. Given two vectors: $\vec{v}_1:(x_1\ y_1\ z_1)$ and $\vec{v}_2:(x_2\ y_2\ z_2)$ .Find the vector $\vec{v}_3=\vec{v}_2\times\vec{v}_1$. What is the physical significance of the vector $\vec{v}_3$?

Hint: The vector $\vec{v}_3$ may be obtained by evaluating the following determinant

$$\begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \end{vmatrix} = \vec{i}\begin{vmatrix} y_1 & z_1 \\ y_2 & z_2 \end{vmatrix} - \vec{j}\begin{vmatrix} x_1 & z_1 \\ x_2 & z_2 \end{vmatrix} + \vec{k}\begin{vmatrix} x_1 & y_1 \\ x_2 & y_2 \end{vmatrix},$$

where $\vec{i}$, $\vec{j}$ and $\vec{k}$ are the unit vectors along the *x*,*y* and *z*-axis, respectively.

W8_4. Given four points: $P:(x_1\ y_1\ z_1)$, $Q:(x_2\ y_2\ z_2)$, $R:(x_3\ y_3\ z_3)$ and $S:(x_4\ y_4\ z_4)$. Find the dihedral angle constituted by these four points.

Hint:

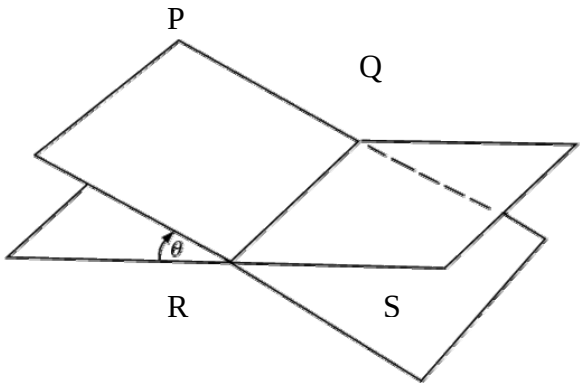
1. Find the components of the vectors PQ, RQ and SR . Here, for the vector PQ, say, its x-component is $x_1 - x_2$.
2. Find the unit normal, U_1 perpendicular to the two vectors PQ and QR by taking their cross product: $\vec{U}_1 = \dfrac{PQ \times QR}{|PQ \times QR|}$
3. Find the unit normal, U_2 perpendicular to the two vectors QR and SR by taking their cross product: $\vec{U}_2 = \dfrac{QR \times SR}{|QR \times SR|}$
4. Obtain the dihedral angle θ as the angle between the two vectors $\vec{U}_1$ and $\vec{U}_2$.

Suggested structure of the program:

1. Read as input the coordinates of the four points as four arrays: r1(3),r2(3),r3(3) and r4(3)
2. Calculate the components of the vectors PQ, QR and SR. For example,

   pq (1) = r1 (1) - r2 (1)
   pq (2) = r1 (2) - r2 (2)
   pq (3) = r1 (3) - r2 (3)

3. Obtain the components of $\vec{U}_1$ and $\vec{U}_2$



W8_5. From our knowledge of chemistry, the molecular geometry is known in terms of bond length, bond angle and dihedral angles. So it is necessary that we convert this knowledge into Cartesian coordinates for further analysis (such as solving Schrodinger equation to obtain the energy eigen values and eigen functions). Using your internet browser, go to the following link:

http://www.shodor.org/chemviz/zmatrices/babel.html

Use this link to obtain the Cartesian coordinates of the following molecules:

(i) water, (ii) acetaldehyde (iii) 1,3-butadiene, (iv) benezene, (v) naphthalene.

In each case, save the resulting coordinates in a separate file; e.g. save the coordinates of water in a file called water.coord.

W8_6.. Write a program that reads in such a coordinate file and gives an output in the PDB format.

W8_7. Use any standard visualization program that runs in linux to visualize the output.