# Assignment I

# CH603

# Molecular Geometry and Rotational Constant Analysis

1. **Read the molecular cartesian coordinates and atomic numbers from the given file.**

Hint 1: Opening and closing the file

Hint 2: Reading the number of atoms

Hint 3: Storing the z-values and the coordinates

2. **Calculate all possible interatomic distances, Ri j.**



Hint 1: Memory allocation

Hint 2: Loop structure

Hint 3: Printing the results

3. **Calculate all possible bond angles. For example, the angle,  , between atoms i−j−k, where j is the central atom is given by:**



**where the eij are unit vectors between the atoms, e.g.,**

   

Hint 1: Memory allocation

Hint 2: Avoiding a divide-by-zero

Hint 3: Memory allocation for the bond angles

Hint 4: Printing only unique non-zero angle

4. **Calculate all possible out-of-plane angles. For example, the angle for atom i out of the plane containing atoms j−k−l (with k as the central atom) is given by:**



Hint 1: Decide do we need to store it.

Hint 2: Calculation of Cross products

Hint 3: Take care of the numerical precision to make sure that sin functions can only have values from -1.0 to +1.0

Hint 4. need to exclude ijkl combinations involving coincidences among the indices as well as distant atom pairs:

5. Calculate all possible torsional angles. For example, the torsional angle  for the atom connectivity i−j−k−l is given by:



Can you also determine the sign of the torsional angle?

Hint 1: Decide do we need to store it.

Hint 2: Take care of the numerical precision to make sure that sin functions can only have values from -1.0 to +1.0

Hint 3. Print only the unique dihedral angles and limit the printing only to atom pairs that are close together.

6. **Find the center of mass of the molecule**

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**where mi is the mass of atom i and the summation runs over all atoms in the molecule**

Hint 1: An excellent source for atomic masses and other physical constants is the [National Institute of Standard and Technology (NIST) website](http://physics.nist.gov/cgi-bin/Compositions/stand_alone.pl?ele=&ascii=html&isotype=some).

Hint 2: Use the masses of the most abundant isotope of each element

7. **Calculate elements of the moment of inertia tensor.**





**where  ,  , and  correspond to choices of x, y, and z (e.g.,  is one choice of  ).**

8. **Diagonalize the inertia tensor to obtain the principal moments of inertia.**

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Hint 1: Use numpy for diagonalization

9. **Determine the molecular type:**

**• diatomic**

**• linear polyatomic**

**• asymmetric top**

**• symmetric top (prolate or oblate)**

**• spherical top**

10**. Determine the moments of inertia in amu.Å2 and g.cm2 and determine the rotational constants in cm−1 and MHz.**



  

*test input and sample output can be found in the input and output directory. For more information see E.B. Wilson, J.C. Decius, and P.C. Cross, ‘Molecular Vibrations’, McGraw-Hill, 1955.*

*(Adapted from https://crawford.chem.vt.edu)*