Geometry Analysis Program

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Goals: Write a computer program to take a set of atomic symbols and Cartesian coordinates for a collection of atoms and determine all possible interatomic distances and bond angles. Assume the coordinates are provided in Angstroms.

Procedure:

1. Read in Cartesian coordinates from an ASCII file in the so-called XYZ format. The first line of this file is just an integer telling how many atoms there are in the file. Each subsequent row i contains an atomic symbol (e.g., C, N, O) and a set of coordinates (x_i, y_i, z_i) for atom i.

2. Calculate all possible interatomic distances

$$R_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}. \tag{1}$$

3. Calculate all possible bond angles between atoms i, j, and k:

$$\begin{aligned} R_{ik}^2 &= R_{ij}^2 + R_{jk}^2 - 2R_{ij}R_{jk}cos\phi_{ijk}, & (2)\\ cos\phi_{ijk} &= \hat{r}_{ji} \cdot \hat{r}_{jk}, & (3) \end{aligned}$$

where

$$\vec{r}_{ij} = (x_j - x_i)\hat{i} + (y_j - y_i)\hat{j} + (z_j - z_i)\hat{k} \tag{4}$$

For additional challenge, try the following: Define unit vectors $\hat{e}_{ij}$ pointing in the direction between atoms i and j, as

$$\hat{e}_{ij} = \vec{r}_{ij}/R_{ij}. \tag{5}$$

1. Calculate all possible out-of-plane angles,

$$sin\theta_{ijkl} = \frac{\hat{e}_{lj} \times \hat{e}_{lk}}{sin\theta_{jlk}} \cdot \hat{e}_{li} \tag{6}$$

2. Calculate all possible torsional angles,

$$cos\tau_{ijkl} = \frac{(\hat{e}_{ij} \times \hat{e}_{jk}) \cdot (\hat{e}_{jk} \times \hat{e}_{kl})}{sin\phi_{ijk} sin\phi_{jkl}}. \tag{7}$$

3. Find the center of mass of the molecule.

$$X_{c.m.} = \frac{\sum_i m_i x_i}{\sum_i m_i}, \tag{8}$$

$$Y_{c.m.} = \frac{\sum_i m_i y_i}{\sum_i m_i}, \tag{9}$$

$$Z_{c.m.} = \frac{\sum_i m_i z_i}{\sum_i m_i}. \tag{10}$$

4. Shift the atomic coordinates to the new center-of-mass reference frame.

5. Calculate the elements of the moment of inertia tensor

$$I_{\alpha\alpha} = \sum_i m_i \left(\beta_i^2 + \gamma_i^2\right), \tag{11}$$

$$I_{\alpha\beta} = -\sum_i m_i \alpha_i \beta_i, \tag{12}$$

   where α, β, γ are Cartesian coordinates in the new center-of-mass frame.

6. Diagonalize the moment of inertia tensor to obtain the principal moments of inertial. You can find a matrix diagonalizer in the PSI libraries on in the BLAS libraries.

$$I_a \leq I_b \leq I_c. \tag{13}$$

7. Determine the molecular type

   (a) diatomic

   (b) linear

   (c) asymmetric top

   (d) symmetric top (oblate or prolate)

   (e) spherical top

8. Determine the rotational constants in cm^{-1} and MHz.

$$A \geq B \geq C, \tag{14}$$

$$A = \frac{h}{8\pi^2 I_a}, \tag{15}$$

$$B = \frac{h}{8\pi^2 I_b}, \tag{16}$$

$$C = \frac{h}{8\pi^2 I_c}. \tag{17}$$

Additional Information: See *Molecular Vibrations*, E. Bright Wilson, J. C. Decius, and Paul C. Cross (Dover, New York, 1980).

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