

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

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

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

$$R_{ik}^2 = R_{ij}^2 + R_{jk}^2 - 2R_{ij}R_{jk}\cos\phi_{ijk}, \quad (2)$$

$$\cos\phi_{ijk} = \hat{r}_{ji} \cdot \hat{r}_{jk}, \quad (3)$$

where

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

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

$$\hat{e}_{ij} = \vec{r}_{ij}/R_{ij}. \quad (5)$$

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

$$\sin\theta_{ijkl} = \frac{\hat{e}_{ij} \times \hat{e}_{lk}}{\sin\theta_{jlk}} \cdot \hat{e}_{li} \quad (6)$$

2. Calculate all possible torsional angles,

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

3. Find the center of mass of the molecule.

$$X_{c.m.} = \frac{\sum_i m_i x_i}{\sum_i m_i}, \quad (8)$$

$$Y_{c.m.} = \frac{\sum_i m_i y_i}{\sum_i m_i}, \quad (9)$$

$$Z_{c.m.} = \frac{\sum_i m_i z_i}{\sum_i m_i}. \quad (10)$$

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

5. Calculate the elements of the moment of inertia tensor

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

$$I_{\alpha\beta} = -\sum_i m_i \alpha_i \beta_i, \quad (12)$$

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 inertia. You can find a matrix diagonalizer in the PSI libraries or in the BLAS libraries.

$$I_a \leq I_b \leq I_c. \quad (13)$$

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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