Dipole moments

Dipole moments occur when there is a separation of charge. They can occur between two ions in an ionic bond or between atoms in a covalent bond; dipole moments arise from differences in electronegativity. The larger the difference in electronegativity, the larger the dipole moment. The distance between the charge separation is also a deciding factor in the size of the dipole moment. The dipole moment is a measure of the polarity of the molecule.

Introduction

When atoms in a molecule share electrons unequally, they create what is called a dipole moment. This occurs when one atom is more electronegative than another, resulting in that atom pulling more tightly on the shared pair of electrons, or when one atom has a lone pair of electrons and the difference of electronegativity vector points in the same way. One of the most common examples is the water molecule, made up of one oxygen atom and two hydrogen atoms. The differences in electronegativity and lone electrons give oxygen a partial negative charge and each hydrogen a partial positive charge.

Dipole Moment

When two electrical charges, of opposite sign and equal magnitude, are separated by a distance, an electric dipole is established. The size of a dipole is measured by its dipole moment (μ). Dipole moment is measured in Debye units, which is equal to the distance between the charges multiplied by the charge. The dipole moment of a molecule can be calculated by:

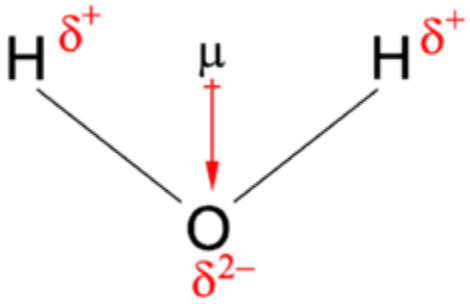
$$\vec{\mu} = \sum_{i} q_i \vec{r}_i$$

Where μ is the dipole moment vector

q is the magnitude of the charge, and

r is the vector representing the position of charge.

The dipole moment acts in the direction of the vector quantity. An example of a polar molecule is H2O. Because of the lone pair on oxygen, the structure of H2O is bent. Hence, water is polar.



Short Instructions for Dipole Moment Calculations

Overview

The dipole.tcl script calculates the dipole moment of a protein using a DCD trajectory file. For each frame in the trajectory, the script outputs the dipole moment components in the x, y, and z directions. The number of lines in the dipole output file corresponds to the number of frames in the trajectory.

Dipole Command

The dipole command computes the dipole moment vector of selected atoms based on their positions and charge values. Here are the options you can use:

- -elementary: Assumes charges are in units of an elementary charge and distances are in angstroms. Output is in the same units by default.
- -debye: Converts the output to units of Debye.
- -geocenter: Uses the geometrical center of the selection as the center of the charge distribution (default).
- -masscenter: Uses the selection's center of mass as the center of the charge distribution. Recommended if the mass values are correctly set for all atoms.

- -origincenter: Uses the origin as the center of the charge distribution.
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Running the Script

The run_dipole.pbs file can be used to run the dipole.tcl script. This file requires two input files:

1. **DCD file**: ./2500Frames/1ubqNVT.dcd (relative path to the DCD file)
2. **PSF file**: ./molPdbPsf/1ubq.psf (relative path to the PSF file)

Making the Script Executable

To make the shell script executable, use the following command in Terminal:

In your bash terminal type and then press Enter:
chmod +x run_dipole.pbs

Running the Script

After making the script executable, you can run it in Terminal:

In your bash terminal type and then press Enter:
./run_dipole.pbs

Output

The output file will be available in the dipoleProtein folder.