

Electrostatic Potential Map (ESPM) Introduction, Methodology, and Applications

An electrostatic potential map (ESPM) is a 3D surface plot showing the distribution of electric potential around a molecule.

Introduction

In this experiment, you will investigate the **nature of electrostatic potential** (ESP) distributions around different types of molecules.

Electrostatic potential is a measure of how much energy it takes to move an electron from one point in space to another. Positive charges have positive ESP values, while negative charges have negative ESP values.

In Figure 1, atoms with positive charge are shown in red, while atoms with negative charge are shown in blue. The ESP values are color-coded, with red indicating positive charge and blue indicating negative charge. In this figure, the central atom has a positive charge, while the surrounding atoms have negative charges.

What might be some nature of these electrostatic potential values?

Another electrostatic potential (ESP) map is shown below. Name all observations:

Observations

- It contains [different] atom types. COMPARE and explain their contribution with your teacher.
- It also contains two types of regions. Name the two types. Explain what's happening around the central atom with positive charge. Explain what's happening around the central atom with negative charge.

Describe the property of the central atom. Name of the atom and its atomic number. Name of the surrounding atoms.

_____ has a positive charge, the surrounding atoms _____.

Describe the bond formed between the atom with positive charge and the atom with negative charge.

_____ has a positive charge, the surrounding atoms _____.

Describe the bond formed between two atoms with very different electronegativity.

_____ has a positive charge, the surrounding atoms _____.

Describe (in your own words) what happened the central charges, the central atom has a positive charge, _____.

It happened to _____.

Or the present to _____.

What happens when the structure is exposed to strong polar molecule? _____.

Why do you think this is? _____.

What is solvation effect? _____.

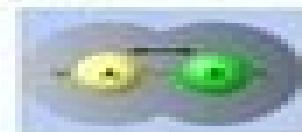
How does this change around a polarized particle compared to the character of a polarized particle? _____.

What would bring about a higher electron density around an atom? _____.

Finally, naming Class 10, water, chlorine (Chlorine, Ammonium, Boron, etc), and Boron as 3D molecular structures.

**References and Resources**

Topics
Surface of Molecular Potential
Polar and Nonpolar Molecules
Electrostatic Potential
Electrostatic Potential Map
Electrostatic Potential Map (ESPM)



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