

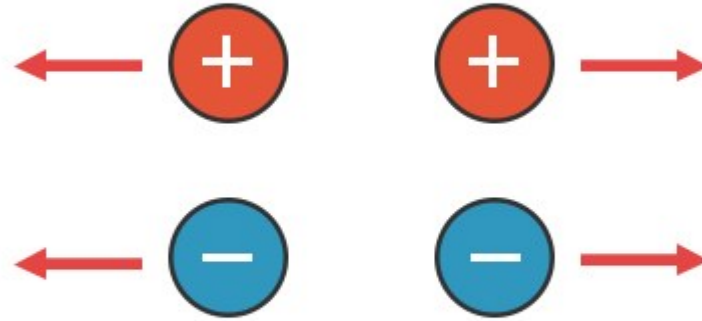
Electrostatic Forces

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- Electrostatic forces are attractive or repulsive forces between particles that are caused by their electric charges. This force is also called the Coulomb force or Coulomb interaction and is so named for French physicist Charles-Augustin de Coulomb, who described the force in 1785.

Electrostatic Force

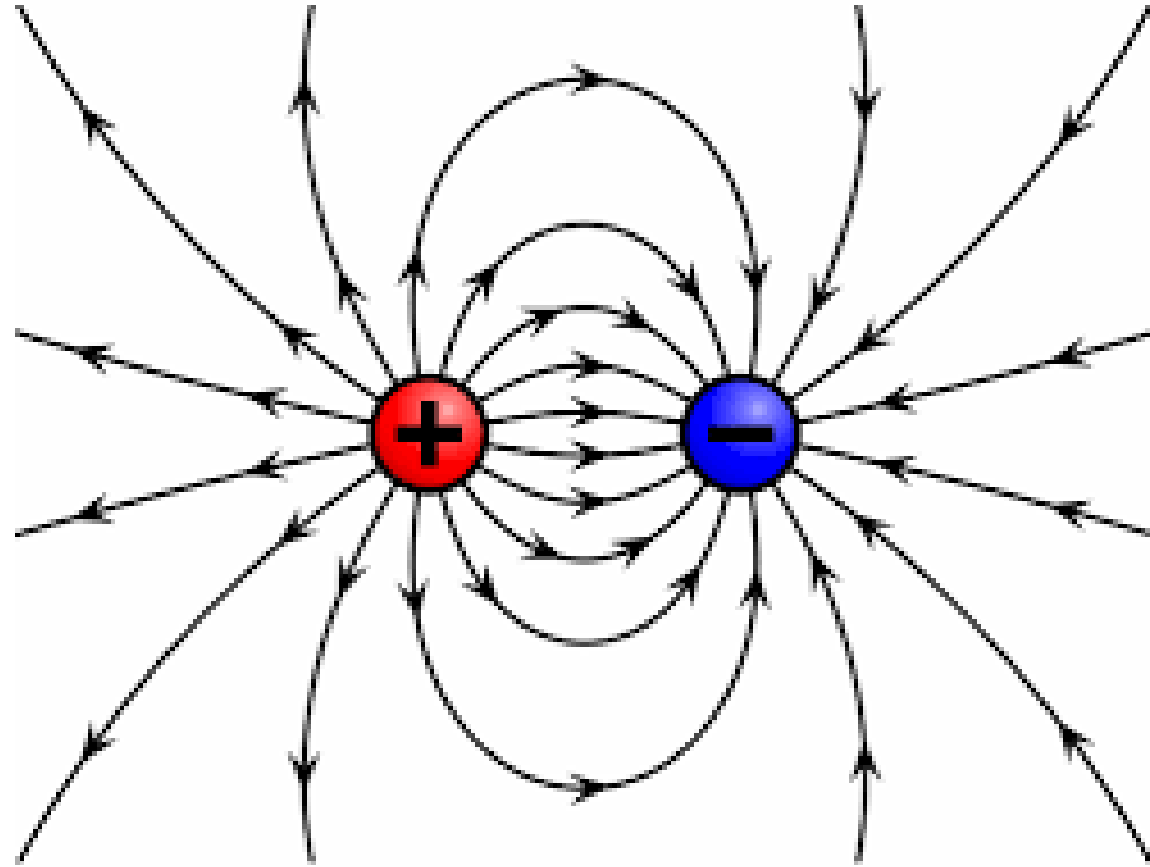
Like charges repel



Opposite charges attract



How the Electrostatic Force Works

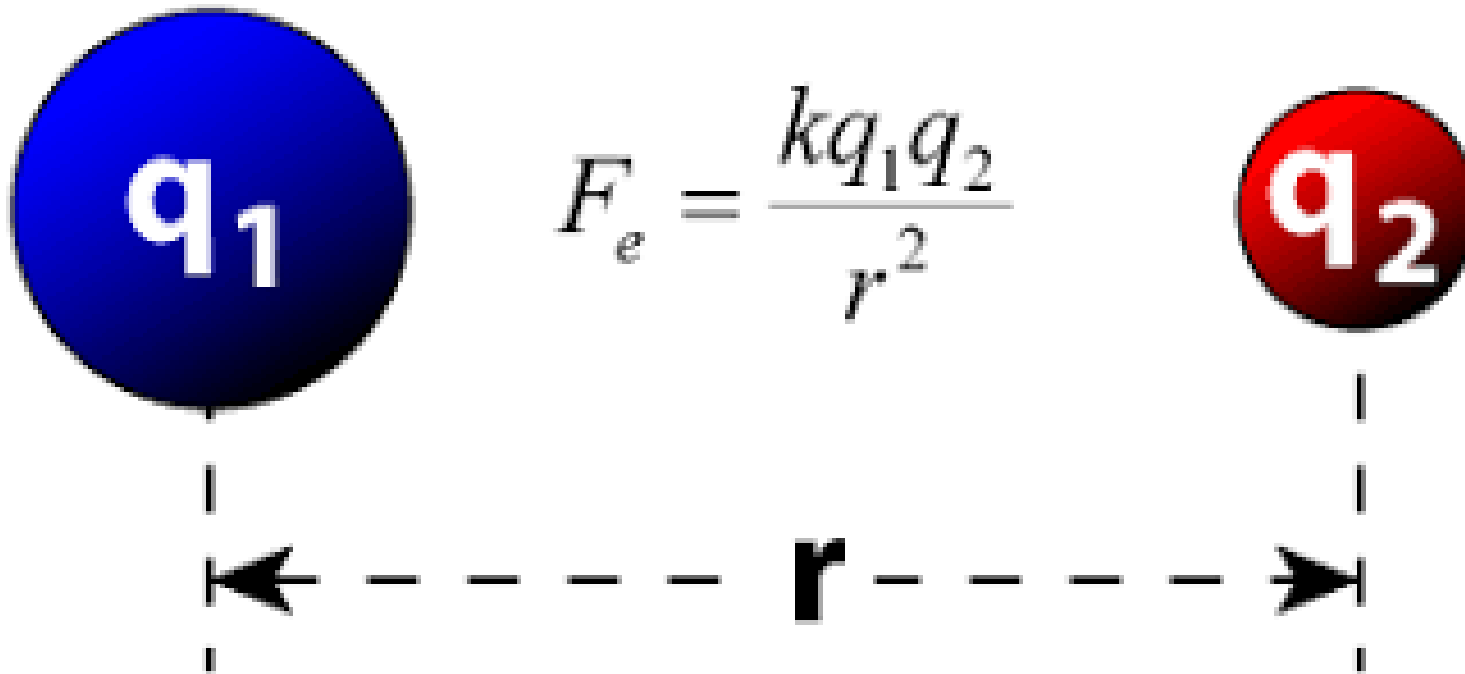


- The electrostatic force acts over a distance of about one-tenth the diameter of an atomic nucleus or 10^{-16} m. Like charges repel one another, while unlike charges attract one another. For example, two positively charged protons repel each other as do two cations, two negatively charged electrons, or two anions. Protons and electrons are attracted to each other and so are cation and anions.
- While protons and electrons are attracted by electrostatic forces, protons don't leave the nucleus to get together with electrons because they are bound to each other and to neutrons by the strong nuclear force. The strong nuclear force is much more powerful than the electromagnetic force, but it acts over a much shorter distance.
- In a sense, protons and electrons are touching in an atom because electrons have properties of both particles and waves. The wavelength of an electron is comparable in size to an atom, so electrons can't get closer than they already are.

Calculating the Electrostatic Force Using Coulomb's Law

- The strength or force of the attraction or repulsion between two charged bodies can be calculated using Coulomb's law:
- $F = kq_1q_2/r^2$
- Here, F is the force, k is proportionality factor, q_1 and q_2 are the two electric charges, and r is the distance between the centers of the two charges. In the centimeter-gram-second system of units, k is set to equal 1 in a vacuum. In the meter-kilogram-second (SI) system of units, k in a vacuum is 8.98×10^9 newton square meter per square coulomb. While protons and ions have measurable sizes, Coulomb's law treats them as point charges.
- It's important to note the force between two charges is directly proportional to the magnitude of each charge and inversely proportional to the square of the distance between them.

Calculating the Electrostatic Force Using Coulomb's Law

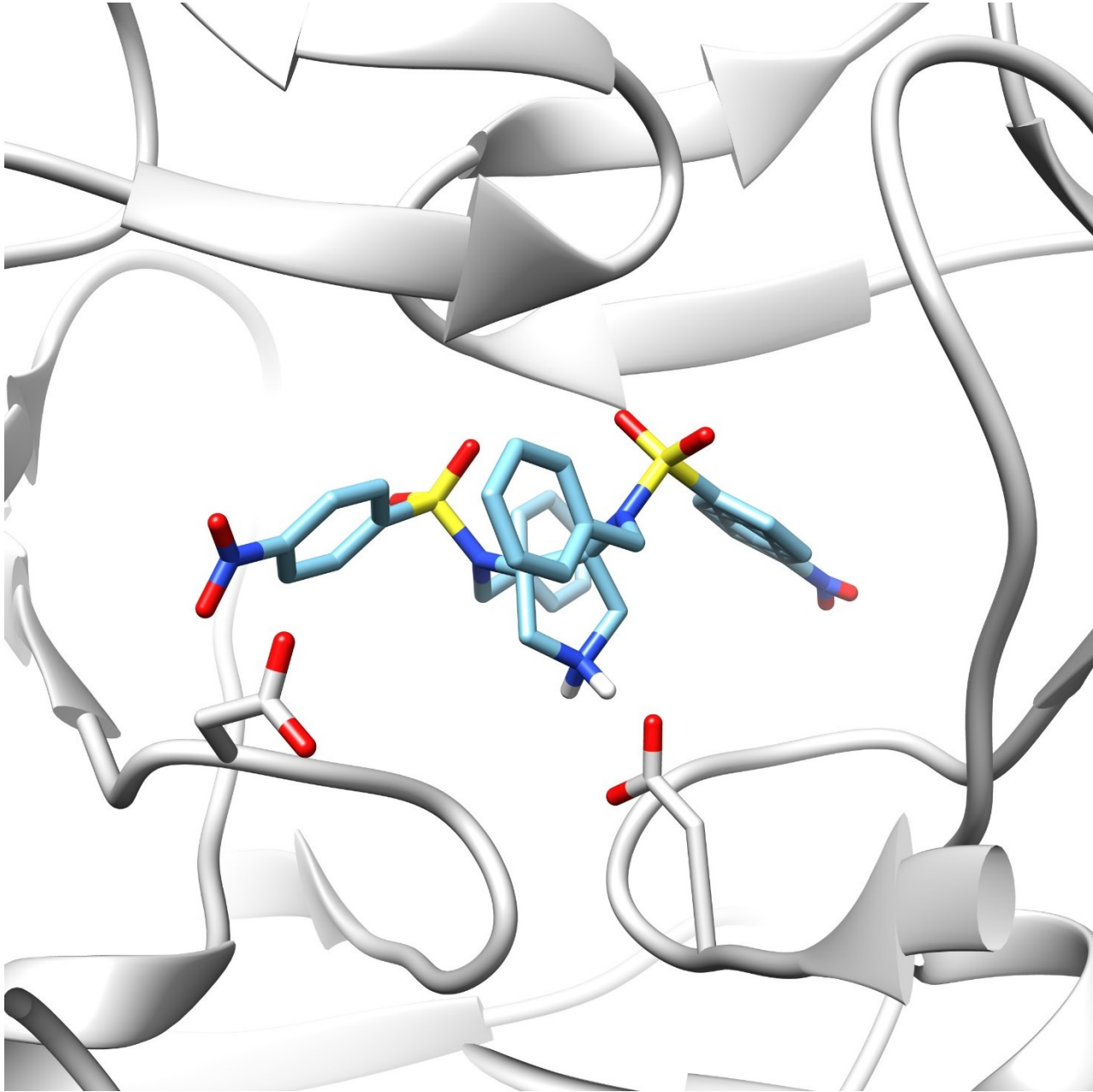


Electrostatics in protein binding and function

- Protein electrostatic properties stem from the proportion and distribution of polar and charged residues. Polar and charged residues regulate the electrostatic properties by forming short range interactions, like salt-bridges and hydrogen-bonds, and by defining the over-all electrostatic environment in the protein.

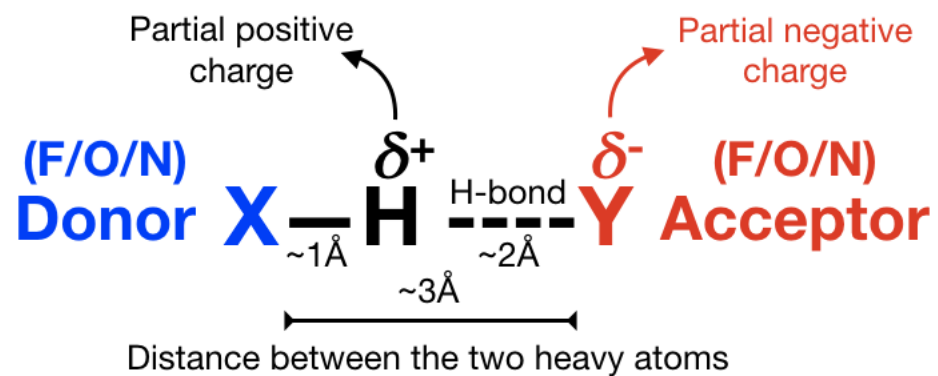
Salt bridge

- A salt bridge can be defined as an interaction between two groups of opposite charge in which at least one pair of heavy atoms is within hydrogen bonding distance.
- A salt bridge is generally considered to exist when the centers of charge are 4 Å or less apart.

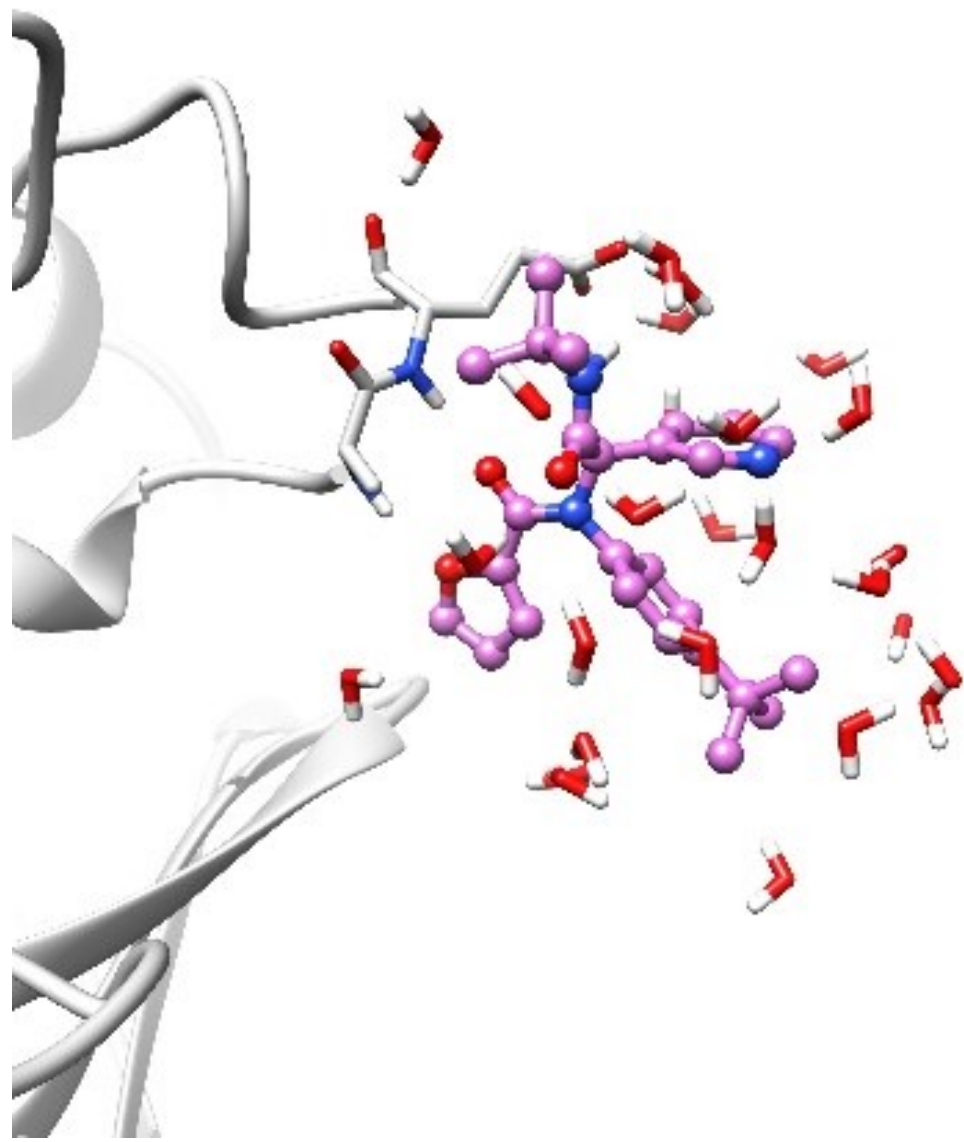


Hydrogen bond

- In chemistry, a hydrogen bond (or H-bond) is a primarily electrostatic force of attraction between a hydrogen (H) atom which is covalently bound to a more electronegative "donor" atom or group (Dn), and another electronegative atom bearing a lone pair of electrons—the hydrogen bond acceptor (Ac). Such an interacting system is generally denoted $Dn-H \cdots Ac$, where the solid line denotes a polar covalent bond, and the dotted or dashed line indicates the hydrogen bond. The most frequent donor and acceptor atoms are the second-row elements nitrogen (N), oxygen (O), and fluorine (F).
- The hydrogen bond (HB) is a chemical concept that was introduced in the 1920s
- For hydrogen bonds, the distance between donor and acceptor atoms is usually 2.7-3.3 Angstroms.



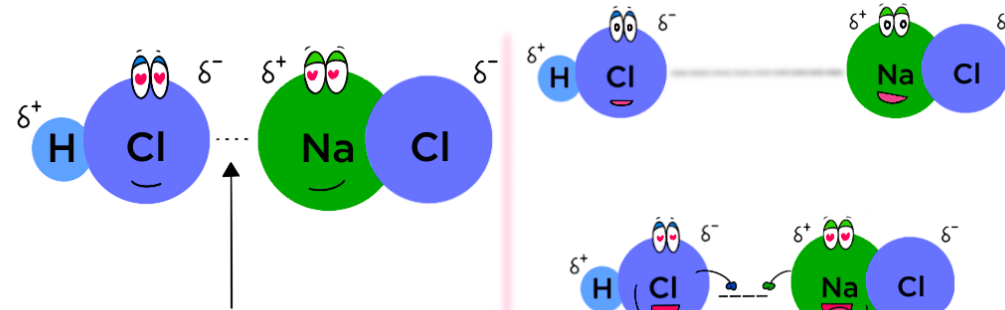
H-bonds	Approximate distance between the heavy atoms
O—H ⋯ O	2.70 ± 0.10
O—H ⋯ O ⁻	2.63 ± 0.10
O—H ⋯ N	2.88 ± 0.13
N—H ⋯ O	3.04 ± 0.13
N ⁺ —H ⋯ O	2.93 ± 0.10
N—H ⋯ N	3.10 ± 0.13



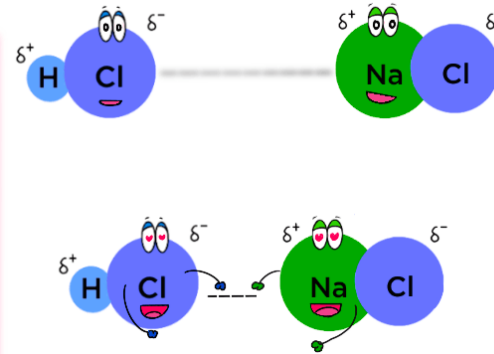
van der Waals Interactions

- Van der Waals interactions occur when adjacent atoms come close enough that their outer electron clouds just barely touch. This action induces charge fluctuations that result in a nonspecific, nondirectional attraction. These interactions are highly distance dependent, decreasing in proportion to the sixth power of the separation. The energy of each interaction is only about 4 kJ mol⁻¹.
- Hydrophobic interactions (van der Waals bonds) have carbon-carbon distances a bit longer, usually 3.3-4.0 Angstroms. In 1873s

What are Van Der Waals (VDW) Forces



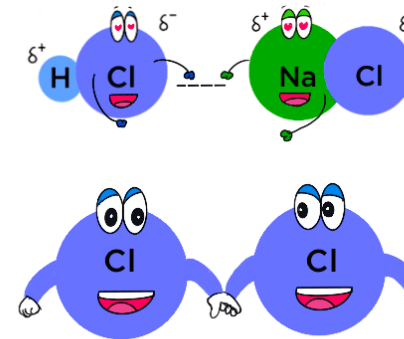
VDW forces are
intermolecular
forces



Distance affects
their strength

Strong
↑
Hydrogen Bonding
Dipole-Dipole
Interaction
London Dispersion
Forces
↓
Weak

Three types of
VDW forces



VDW forces are
weaker than
intramolecular forces

Are hydrogen bond and van der waals electrostatic interactions?

- vander wall forces are present in between molecules specially while electrostatic force may present in molecule.
- The stability and geometry of a hydrogen-bonded dimer is traditionally attributed mainly to the central moiety $AH\cdots B$, and is often discussed only in terms of electrostatic interactions.
- Hydrogen bonds are electrostatic attractions between a hydrogen bearing a partial, positive charge and another atom (usually O or N) bearing a partial negative charge. These partial opposite charges are a consequence of the relative electronegativity of covalently-bonded atoms.
- Hydrogen bond is defined as weak electrostatic force of attraction between hydrogen and a more electronegative atom such as F, O, N... They aren't even close.

References

- DOI: [10.2174/1389203023380431](https://doi.org/10.2174/1389203023380431)
- DOI: [10.1371/journal.pone.0263200](https://doi.org/10.1371/journal.pone.0263200)
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