Intermolecular Forces [pln18]

Pair interactions between molecules typically consist of a short-range repulsive part and a longer-range attractive part. The two parts produce a minimum interaction potential at some distance (e.g. Lennard-Jones potential). This minimum is interpreted as a bond and the depth as the binding energy.

The short-range repulsion is dominated by electronic Coulomb interaction as described quantum mechanically, involving symmetries and the Pauli principle. The longer-range attractive forces are more diverse in nature, strength, and range. They are commonly described as physical bonds of specific types.

Van der Waals bond: Quantum mechanical charge fluctuations intrinsic to electron wave functions of atoms or molecules produce random electric dipole moments. The fluctuating electric dipoles of adjacent molecules cause (on average) an attractive force. The range of the interaction potential depends on whether the molecules have fixed relative orientation ($\sim r^{-3}$) or are free to rotate ($\sim r^{-6}$). The van der Waals bond is only weakly directional if at all and its strength is comparable to $k_{\mathrm{B}}T$ at room temperature.

Ionic bond: Electronic charge transfer between adjacent atoms produces oppositely charged ions. The resulting Coulomb interaction potential is non-directional, much larger than $k_{\mathrm{B}}T$ at room temperature, and long-ranged ($\sim r^{-1}$). In solution ionic bonds become weaker and shorter-ranged due to screening effects.

Covalent bond: Electrons shared by adjacent atoms produce covalent bonds. Most covalent bonds have strengths similar to ionic bonds, some are weaker but still too strong to be broken by energies of $\mathrm{O}(k_{\mathrm{B}}T)$ at room temperature. Covalent bonds are short-ranged and highly directional.

Metallic bond: Electrons are being shared between many atoms in metallic bonds. These electrons become effectively delocalized. Covalent bonds and metallic bonds are related from a quantum mechanical point of view. Metallic sharing produces electrical conductors and covalent sharing electrical insulators.

Hydrogen bond: Hydrogen atoms as constituents of molecules tend to be electropositive. They have a significant unshielded positive charge. They are attracted to electronegative parts of adjacent molecules. Typical strengths vary between $5k_{\mathrm{B}}T$ and $12k_{\mathrm{B}}T$ at room temperature. In biological macromolecules, hydrogen bonds produce structural stability but are readily counteracted by molecular agents or environmental changes.