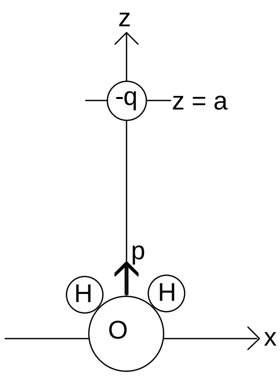
Lisa Larrimore – Physics 112

Dipole Interactions and Biophysics

Biophysicist attempt to use the laws of physics to explain biological phenomena on a molecular scale, and one of the most important parts of this process is understanding intermolecular forces. To examine the role that dipoles play in these forces, let's start with something simple. First, we shall examine the strength of dipole interactions by considering the dipole moment $\vec{p} = p\hat{z}$ separated from a charge -*q* by a distance *a*, as shown below. (This is Purcell 10.18.)

The potential energy of this configuration can be calculated by finding the force on *q* due to the electric field of the dipole:



$$\vec{E}_{dip} = \frac{2p}{z^3}\hat{z} \quad \Rightarrow \quad \vec{F}_q = -\frac{2pq}{z^3}\hat{z}$$

$$\Rightarrow \quad W = \int_a^{\infty} \frac{2pq}{z^3} dz = \frac{pq}{a^2}$$

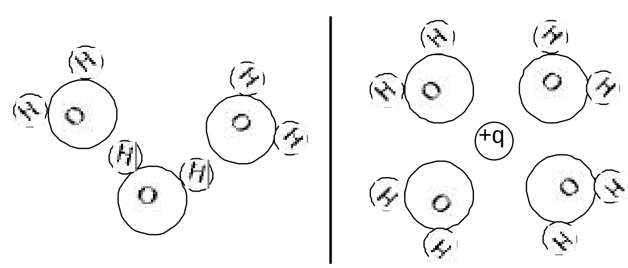
Note that we get the same answer if we find the force on the dipole due to the electric field of q:

$$\vec{E}_q = \frac{q}{(z-a)^3}\hat{z} \quad \Rightarrow \quad \vec{F}_{dip} = (\vec{p}\cdot\nabla)\vec{E} = p\frac{d\vec{E}}{dz} = \frac{-2pq}{(z-a)^3}\hat{z}$$

$$\Rightarrow \quad W = \int_0^{-\infty} \frac{2pq}{(z-a)^3 dz} = \frac{pq}{a^2}$$

Suppose the dipole is a water molecule, so $p = 1.84 \times 10^{-18}$ esu-cm $= 6.13 \times 10^{-30}$ C-m, and the charge -*q* is an electron (or an ion of charge –e), so $q = 4.803 \times 10^{-10}$ esu, and they are separated by a distance $a = 1.5$ Å. Then the potential energy is 3.9×10^{-12} erg, or **2.4 eV**.

For comparison, the potential energy of two H_2O molecules with parallel dipole moments separated by the same distance is $\mathbf{2p^2/a^3 = 1.25}$ **eV**, and the potential energy of two charges, +*q* and –*q*, separated by *a* is $\mathbf{q^2/a = 9.6}$ **eV** if q is the charge of an electron. Note the dependence on *a*: the energy of dipole interactions drops off more quickly than monopole interactions, as we expect. There are also weaker interactions involving induced dipoles and ions, ($W \sim 1/a^4$), permanent dipoles ($W \sim 1/a^6$), and other induced dipoles ($W \sim 1/a^6$).[1]



Note the orientation of the water molecule near the charge. When the dipole is not pointing towards the charge, it feels a torque, $\vec{t} = \vec{p} \times \vec{E}_q$, which forces it to the current stable angular equilibrium. (There is also no torque when the dipole is pointing away from the charge, but this is an unstable equilibrium.) So we see that *ions orient dipoles*. A water molecules generally orients itself to have its more electronegative oxygen atom near the

[1] These energy values are only true in the absence of motion. If undergoing Brownian motion (random bombardment by surrounding molecules), ion-dipole energy scales like $1/r^4$ and dipole-dipole energy scales like $1/r^6$. (See Daune *Molecular Biophysics* 1999.)

hydrogen atoms of other water molecules, but if you place an positive ion in water, the force aligning the dipoles with the E-field of the ion is stronger than the force aligning them with each other, as shown.

(hand-drawn picture of potassium channel)

One interesting application of dipoles in biophysics involves the motion of potassium through **ion channels** in cell membranes.[2] Potassium ions carry a +1 charge, so their interaction with dipoles is similar to that examined above. Ions that are too large to directly penetrate the phospholipid bilayer that makes up your cell membranes are transported from one side to another by being actively pumped through (if they are going against the potential gradient) or by passively going through transport protein channels.

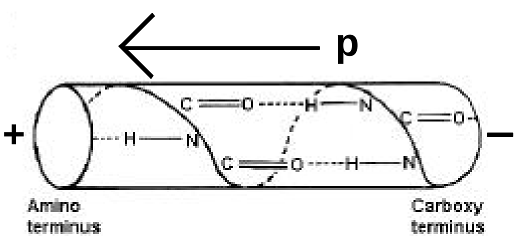
To enter a channel, the potassium ion must move from water, in which the dielectric constant is 80, to a region of lower dielectric constant $e < 80$. This energy barrier is known as the **Born energy**, and it can be found by considering the work it takes to charge a sphere of radius R_B from 0 to q:

$$W = \int dW = \int_0^q \frac{q' dq'}{4pe_0 e R_B} = \frac{q^2}{8pe_0 R_B} \frac{1}{e}$$

The Born energy is then the energy needed to charge the sphere in the channel minus the energy gained by decharging the sphere in water:

$$E_B = \frac{q^2}{8pe_0 R_B}\left(\frac{1}{e} - \frac{1}{80}\right)$$

For potassium, R_B = 1.93 Å, so to give an idea of the size of this energy barrier, if e = 20, 40, or 60, E_B = 5.4 kT, 1.8 kT, or 0.6 kT, respectively. In the absence of any electrostatic forces, potassium atoms will not be able to traverse the channel.



However, the insides of the channel are lined with mouth dipoles, carbonyl groups, and helix dipoles, with dipole moments of 30, 7.2, and 96.3 x 10^{-30} C-m, respectively. A model of an alpha helix dipole is shown at left: the oxygen atoms are near the channel boundaries, and the positive amino terminus is further away from the channel, so the dipole moments point away from the channel. This creates a potential energy well that overcomes the Born energy.

So once a potassium ion is drawn into the potential well created by dipoles inside a channel, why would it exit? If there were just one ion, it wouldn't. It turns out that the potential well is deep enough to hold two ions in a stable configuration. But each ion in the well changes the potential profile seen by other ions (positive ions don't want to be near each other), and so a third ion is drawn to the well and is pulled out the other side by other dipoles. This mechanism results in a current through the ion channel.

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[2] Chung, et al, "Permeation of Ions Across the Potassium Channel: Brownian Dynamics Studies," *Biophysical Journal*, 77, 2517-2533 (November 1999).