
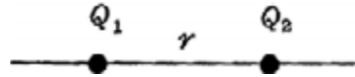
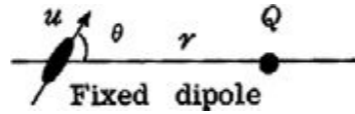
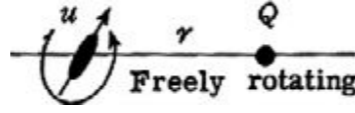
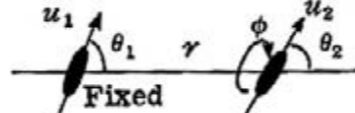
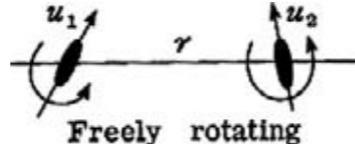
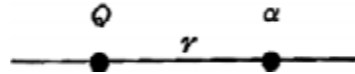
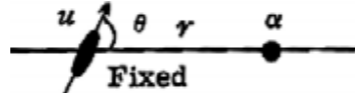
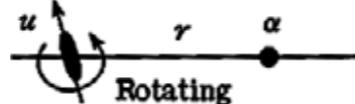
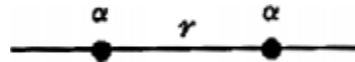
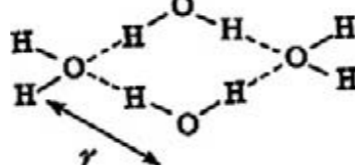


Bonding

Type of interaction		Interaction energy $w(r)$
Covalent, metallic		Complicated, short range
Charge-charge		$+Q_1Q_2/4\pi\epsilon_0r$ (Coulomb energy)
Charge-dipole		$-Qu \cos \theta/4\pi\epsilon_0r^2$
		$-Q^2u^2/6(4\pi\epsilon_0)^2kTr^4$
Dipole-dipole		$-u_1u_2[2 \cos \theta_1 \cos \theta_2 - \sin \theta_1 \sin \theta_2 \cos \phi]/4\pi\epsilon_0r^3$
		$-u_1^2u_2^2/3(4\pi\epsilon_0)^2kTr^6$ (Keesom energy)
Charge-non-polar		$-Q^2\alpha/2(4\pi\epsilon_0)^2r^4$
Dipole-non-polar		$-u^2\alpha(1 + 3 \cos^2 \theta)/2(4\pi\epsilon_0)^2r^6$
		$-u^2\alpha/(4\pi\epsilon_0)^2r^6$ (Debye energy)
Two non-polar molecules		$-\frac{3}{4} \frac{h\nu\alpha^2}{(4\pi\epsilon_0)^2r^6}$ (London dispersion energy)
Hydrogen bond		Complicated, short range, energy roughly proportional to $-1/r^2$

^a $w(r)$ is the interaction free energy or pair-potential (in J); Q , electric charge (C); u , electric dipole moment (C m); α , electric polarizability ($C^2 m^2 J^{-1}$); r , distance between the centers of the interacting atoms or molecules (m); k , Boltzmann constant ($1.381 \times 10^{-23} J K^{-1}$); T , absolute temperature (K); h , Planck's constant ($6.626 \times 10^{-34} J s$); ν , electronic absorption (ionization) frequency (s^{-1}); ϵ_0 , dielectric permittivity of free space ($8.854 \times 10^{-12} C^2 J^{-1} m^{-1}$). The force $F(r)$ is obtained by differentiating the energy $w(r)$ with respect to distance r : $F = -dw/dr$. The stabilizing repulsive "Pauli Exclusion" interactions (not shown) usually follow an exponential function $w(r) \propto \exp(-r/r_0)$, but for simplicity they are usually modeled as power laws: $w(r) \propto +1/r^n$ (where $n = 9-12$).

Type of Bond	Substance	Bond Energy, kJ/mol	Melting Point, (°C)	Characteristics
Ionic	CaCl	651	646	Low electrical conductivity, transparent, brittle, high melting point
	NaCl	768	801	
	LiF	1008	870	
	CuF ₂	2591	1360	
	Al ₂ O ₃	15,192	3500	
Covalent	Ge	315	958	Low electrical conductivity, very hard, very high melting point
	GaAs	~315	1238	
	Si	353	1420	
	SiC	1188	2600	
	Diamond	714	3550	
Metallic	Na	109	97.5	High electrical and thermal conductivity, easily deformable, opaque
	Al	311	660	
	Cu	340	1083	
	Fe	407	1535	
	W	844	3370	
van der Waals	Ne	2.5	-248.7	Weak binding, low melting and boiling points, very compressible
	Ar	7.6	-189.4	
	CH ₄	10	-184	
	Kr	12	-157	
	Cl ₂	31	-103	
Hydrogen bonding	HF	29	-92	Higher melting point than van der Waals bonding, tendency to form groups of many molecules
	H ₂ O	50	0	

The Born Energy

- When we talk about an ion in free space. we are not taking in to account the energy needed to form that ion. We have talked about the Ionisation and electron affinities but there is a second way to define it, the Born Energy of an Ion, here is the derivation.

- We could build this ion by taking an atom and adding charge to it, the instantaneous charge on the ion will be q and the charge we add will be dq

$$dw = \frac{q dq}{4\pi\epsilon\epsilon_0 a}$$

The change in energy dw , when we add charge dq . A is the ion radius

$$u = \int dw = \int_0^Q \frac{q dq}{4\pi\epsilon\epsilon_0 a}$$

The total energy held in this ion is now
This is the energy it takes to form the ion

$$u = \frac{Q^2}{8\pi\epsilon\epsilon_0 a}$$

What happens when we move the ion around

$$\Delta u = \frac{Q^2}{8\pi\epsilon_0 a} \left[\frac{1}{\epsilon_1} - \frac{1}{\epsilon_2} \right]$$

If we move the ion between mediums of different relative permittivity. The energy changes.

If we move the ion from air ($\epsilon=1$) to water ($\epsilon=78$)
Then the change in energy is on the order of 1000 KJ/mol
Which is pretty significant.

This is about 40 times greater than kT .

Solubility

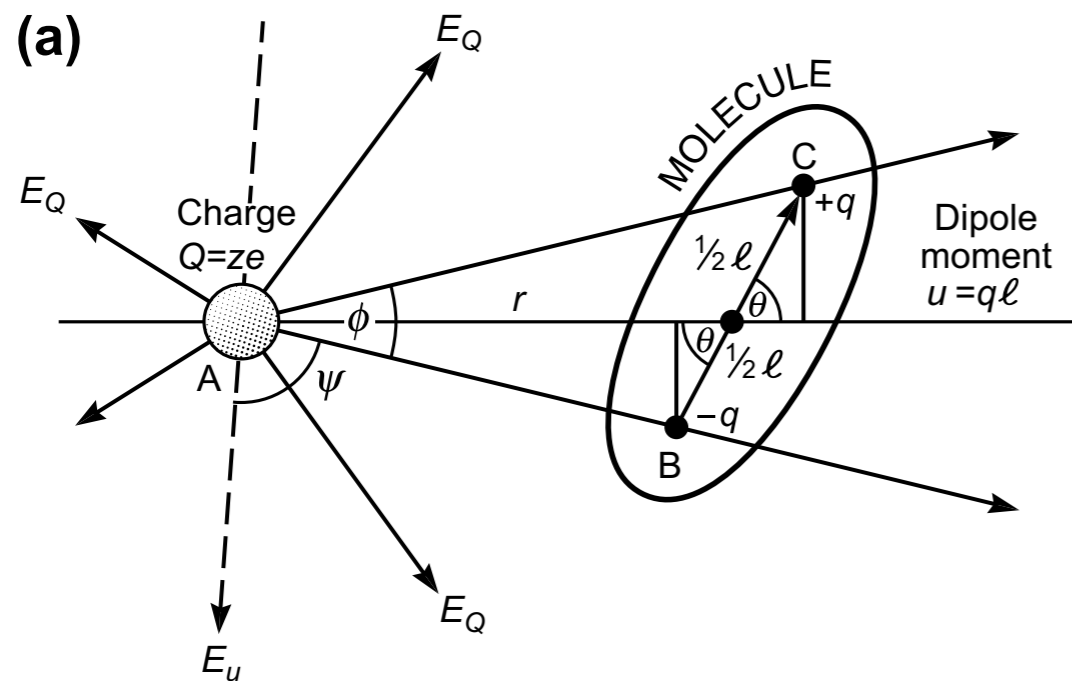
If we think about our ions in water some will have more energy than others. This will be a Boltzmann distribution.

$$X_s = e^{\frac{-\Delta U}{KT}} = e^{-\left(\frac{Q^2}{8\pi\epsilon\epsilon_0(a_+ + a_-)KT}\right)}$$

We can write the as given here, note the a_+ and a_- . These are the radii of the individual ions.

X_s is the solubility of an electrolyte in water, or in any solvent, in mole-fraction units. Thus, for NaCl in water, where $(a_+) + (a_-) = 0.276\text{nm}$, $\epsilon = 78$ at $T = 298\text{K}$, we expect very roughly $X_s = e^{-2.6} = 0.075$ in mole fraction unit, which may be compared with the experimental value of 0.11 mole/mole (360 g/liter).

Dipole Ion interaction



$$U_r = -\frac{Qq}{4\pi\epsilon\epsilon_0} \left[\frac{l}{AB} - \frac{l}{AC} \right]$$

note $U \rightarrow w$ (to stop confusion with dipole moment) : $u=ql$

$$w_r = -\frac{zeu \cos\theta}{4\pi\epsilon\epsilon_0 r^2}$$

Energy landscape

