Practice Problem for Problem S4 of homework #2

Remember that if we choose property A to be a function of B and C, i.e., $A = A(B,C)$, this is equivalent to saying what?:

$$dA = \left( \frac{\partial A}{\partial B} \right)_C dB + \left( \frac{\partial A}{\partial C} \right)_B dC$$

for any state function.
Practice Problem like homework S4

Picking some letters randomly from the alphabet, \( A = A(B, C); \) 
\[ dA = D \ dB + E \ dC \] 
i.e., variables are \( B \) and \( C \) 
and \( D \) and \( E \) are slopes (\( = \) partial derivatives)

This means automatically (no thought required) that

\[ dA = \left( \frac{\partial A}{\partial B} \right)_C dB + \left( \frac{\partial A}{\partial C} \right)_B dC \]

Then it follows that: \( \left( \frac{\partial A}{\partial B} \right)_C = D \) and \( \left( \frac{\partial A}{\partial C} \right)_B = E \)

and James Clerk Maxwell showed that \( \left( \frac{\partial D}{\partial C} \right)_B = \left( \frac{\partial E}{\partial B} \right)_C \)

The \( B \) slope (i.e., \( D \)) changes with \( C \) exactly as the \( C \) slope (i.e., \( E \)) changes with \( B \)
a. **Weak Non-Covalent “Reactions”**

   essential for the *DYNAMICS* of life processes

1. Ionic (in solution or biopolymers),
2. “hydrogen bonding”,
3. hydrophobic *(not)* bonding
4. London dispersion forces
   *(universally present)*

b. proteins: what are they? and what do they do?
All of chemistry is built from **Coulomb’s Law:** The very strong attraction of opposite charges and repulsion of like charges.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Characteristic interaction</th>
<th>$\Delta_f H^\circ$ (kJ mol$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{Na}^+(g) + \text{Cl}^-(g) \rightarrow \text{NaCl}(s)$</td>
<td>Ionic</td>
<td>$-785$</td>
</tr>
<tr>
<td>$\text{NaCl}(s) + \infty \text{H}_2\text{O}(l) \rightarrow \text{Na}^+(aq) + \text{Cl}^-(aq)$</td>
<td>Ionic and ion–dipole</td>
<td>$4$</td>
</tr>
<tr>
<td>Argon($g$) $\rightarrow$ Argon($s$)</td>
<td>London</td>
<td>$-8$</td>
</tr>
<tr>
<td>$n$-Butane($g$) $\rightarrow$ $n$-Butane($l$)</td>
<td>London–van der Waals</td>
<td>$-20$</td>
</tr>
<tr>
<td>Acetone($g$) $\rightarrow$ Acetone($l$)</td>
<td>London–van der Waals</td>
<td>$-30$</td>
</tr>
</tbody>
</table>

**van der Waals:** a **mixture** of London and permanent dipole-dipole interactions
Hydrogen bonding is almost all *electrostatic* attraction of partial charges. It is strong because of **smallness of H; H gets closer than any other atom!**
Hydrogen Bonding

Hydrogen bonding is almost all *electrostatic attraction* of partial charges. It is strong because of *smallness* of H.
IN WATER

\[
\begin{align*}
\text{Urea} & \quad + \quad \text{Urea} \\
\text{(aq)} & \quad \quad \quad \quad \quad \quad \text{(aq)}
\end{align*}
\]

Hydrogen bond
(aqueous) \(-5\)

\[
\begin{align*}
\text{C}_3\text{H}_6(l) & + \infty \text{H}_2\text{O}(l) \rightarrow \text{C}_3\text{H}_6(\text{aq}) \\
\text{Benzene}(l) & + \infty \text{H}_2\text{O}(l) \rightarrow \text{benzene}(\text{aq})
\end{align*}
\]

Hydrophobic \(-10\)

Hydrophobic \(0\)
London dispersion forces

Quantum behavior and \textit{ALWAYS PRESENT regardless of what other label is given to a force}

Electrons in atoms act like \textit{particles}, although the orbital picture makes them seem like spherical clouds with no dipole.

Particle behavior means \textit{helium} atoms have large \textit{fluctuating dipoles}.

Two helium atoms side by side attract because the \textit{fluctuations are correlated to reduce electron repulsion} between the atoms.

\textit{instantaneous dipole-induced dipole}

\begin{align*}
+ & \rightarrow - \\
- & \rightarrow + \\
- & \rightarrow + \quad \text{or} \quad + & \rightarrow -
\end{align*}
Hydrophobic “bonding”, “interactions”, are actually *thermodynamic reactions* that involve all the forces we have introduced.
Soap & Detergent

Hydrocarbon tail

micelle

Na+

Counter Ions

Na+
Biological Soaps = Lipids = Fats.

Form bilayers = membranes.

Water

And vesicles (for transport)

E.g. neural transmitters

Water
Note: The London forces between water and ethane are ~same as between two ethanes. Total ordered water is reduced by association of ethanes. The force is much the same as what causes water droplets in air to be spherical and makes them combine into larger drops, i.e., surface tension. Reducing surface area is spontaneous.
Hydrophobic "Bonding"

AROMATIC RING IN WATER. Typical snapshot showing different views of the H-bonded chains formed by water within 4.0 Angstroms.

10 femtoseconds later
What are proteins and what do they do?

The poetic answer:
"We now see that proteins are highly sophisticated molecular machines that process energy, matter, and information. Their beautiful molecular ballet is coming into view."

-Lubert Stryer

*Biochemistry, 4th Ed.*
What do proteins do? The list answer:

(Gene == basic Protein)

but there are many forms of most basic proteins created by post translational processes

Mechanical support
Motion
Transport and storage
Immune protection
Signaling (nerve impulses, response to hormones, vision,……
Catalysis and recognition-- pervade most of the above
(in particular, hydrolysis of ATP and GTP provides the energy for switching and timing of the complex circuits)

and much, much more—yet to be discovered.
The visual answer

Ecoli Bacterium
Interacting Signaling Pathways

- = ligands

- = PROTEINS
What are proteins? The chemical answer:

- Linear polymers of amino acids
- The sequence is from the genetic code
- ~100,000 proteins are responsible for the life process

Backbone

Sidechains

H on each Cα not shown