- Reading
- Today: pp 80-87
- Thursday: pp 101-104
- Friday pp 104(bottom)-107

Non-Covalent "Reactions"

important for the *DYNAMICS* of life processes

a. Ionic,
"hydrogen bonding",
hydrophobic (not) bonding
London dispersion forces ("spooky")

b. proteins: what are they?
what do they do?

London dispersion forces

Quantum behavior

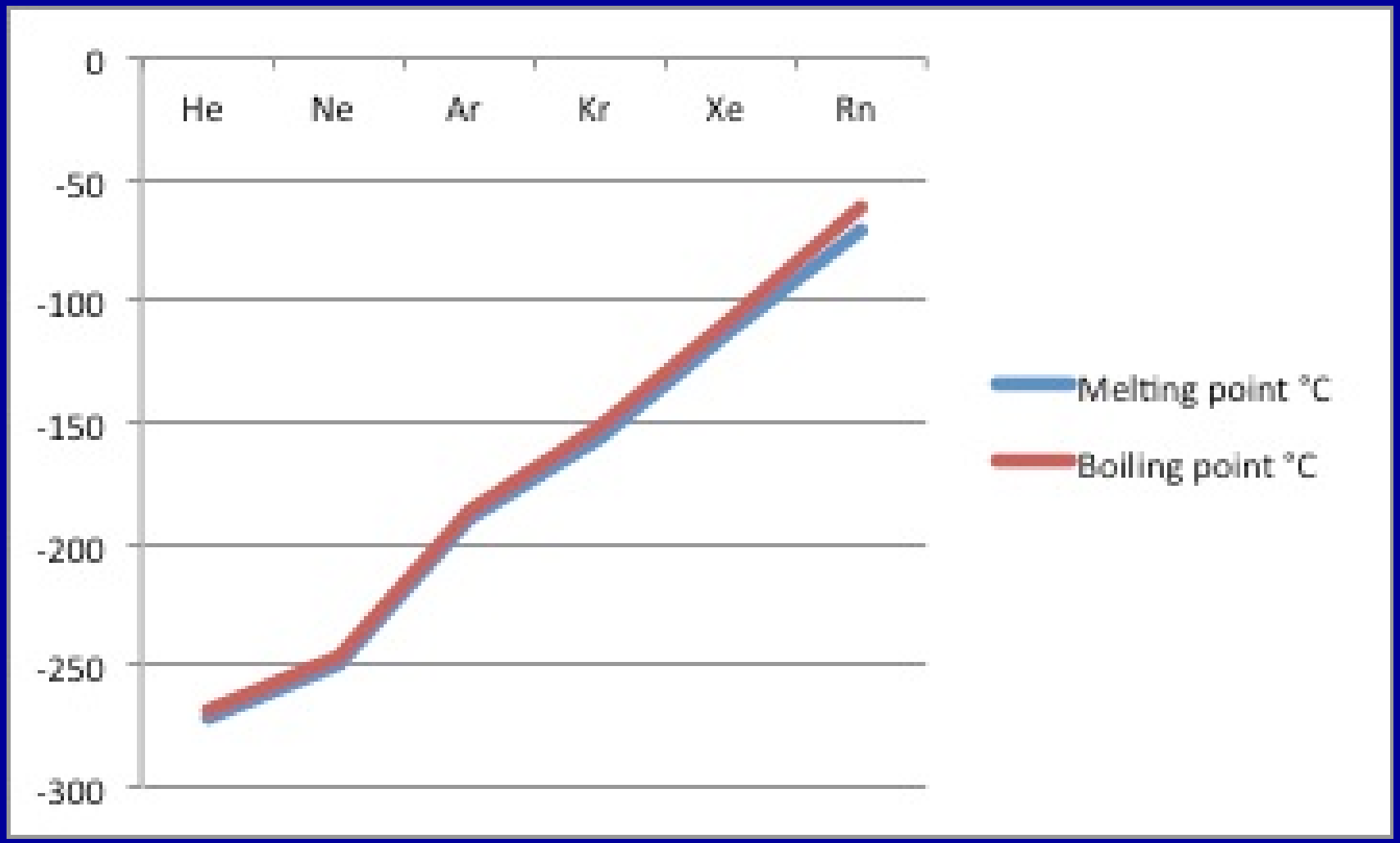
Electrons in atoms act like **particles**, although the orbital picture makes them seem like spherical clouds with no dipole.

Particle behavior means *helium* atoms have **large f*luctuating dipoles.***

Two helium atoms side by side attract because the **fluctuations are correlated to reduce electron repulsion** between the atoms.

instantaneous dipole- induced dipole

+	-		-	+
-	+	***or***	+	-


0
-50
-100
-150
-200
-250
-300
He
Ne
Ar
Kr
Xe
Rn
Melting point °C
Boiling point °C

All of chemistry is built from Coulomb's Law: The very strong attraction of opposite charges and repulsion of like charges.

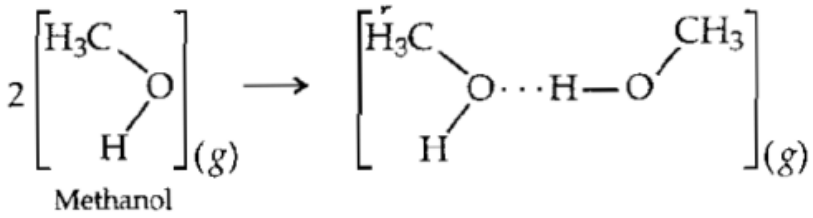
TABLE 3.1 **Enthalpies of Noncovalent Bonds and Interactions***

Reaction	Characteristic interaction	$\Delta_r H°$ (kj mol^{-1})
$Na^+(g) + Cl^-(g) \rightarrow NaCl(s)$	Ionic	−785
$NaCl(s) + \infty H_2O(l) \rightarrow Na^+(aq) + Cl^-(aq)$	Ionic and ion–dipole	4
$Argon(g) \rightarrow Argon(s)$	London	−8
n-Butane$(g) \rightarrow n$-Butane(l)	London–van der Waals	−20
$Acetone(g) \rightarrow Acetone(l)$	London–van der Waals	−30

van der Waals: a ***mixture*** of London and permanent dipole-dipole interactions

Hydrogen Bonding

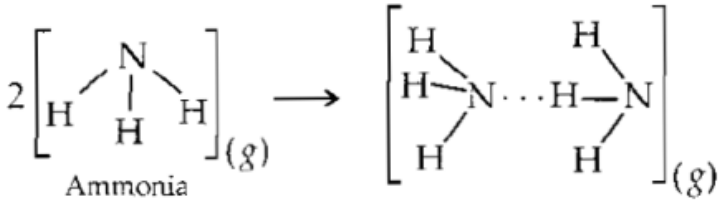
Hydrogen bonding is almost all *electrostatic attraction* of partial charges. It is strong because of *smallness* of H



Methanol

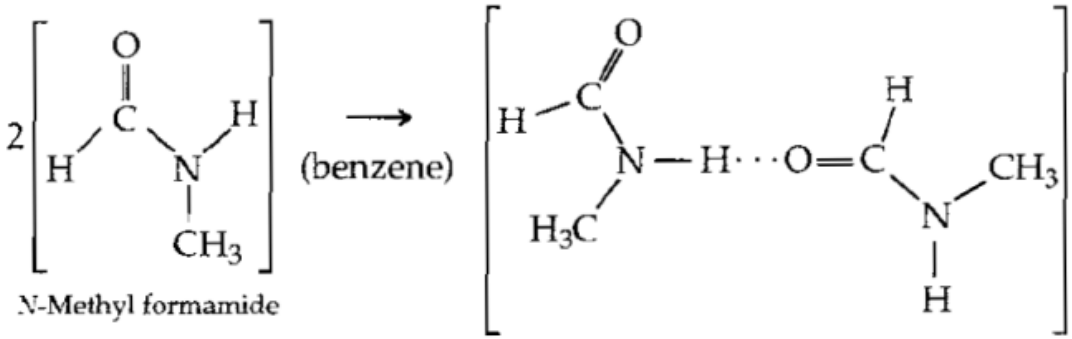
GAS PHASE

Hydrogen bond (*g*) −20



Ammonia

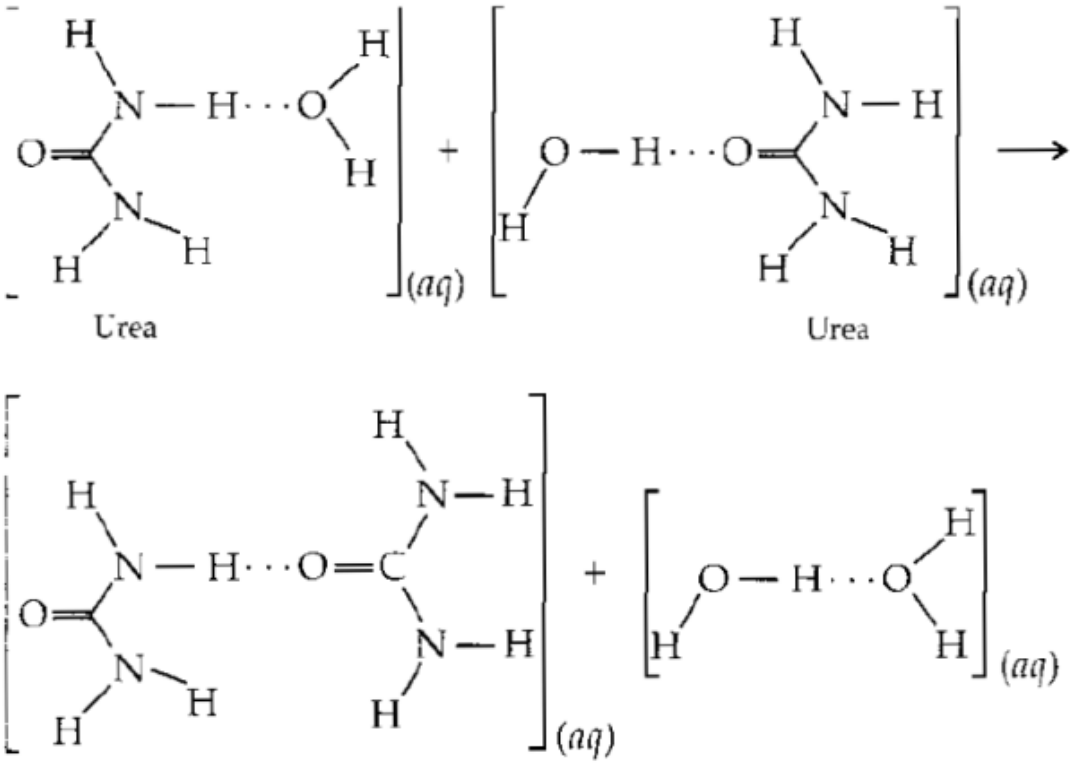
Hydrogen bond (*g*) −15



N-Methyl formamide

Hydrogen bond (benzene) −15

IN WATER



	Hydrogen bond (aqueous)	−5
$C_3H_6(l) + \infty H_2O(l) \rightarrow C_3H_6(aq)$	Hydrophobic	−10
Benzene$(l) + \infty H_2O(l) \rightarrow$ benzene(aq)	Hydrophobic	0

Coulombic Terms (electrostatic)

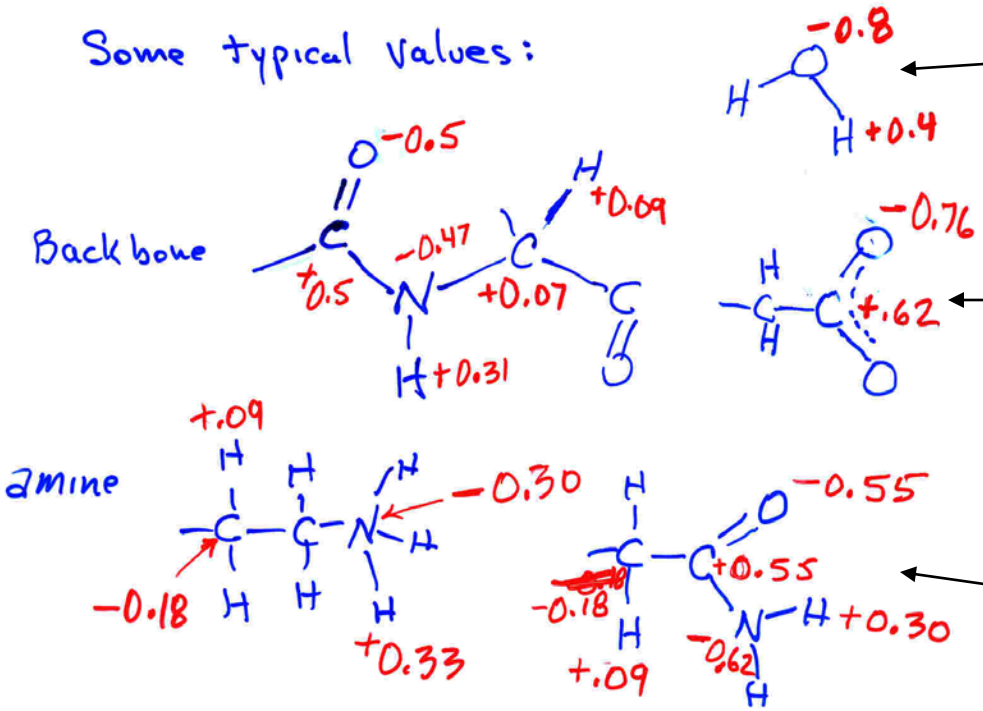
$$(V_{coul})_{ij} = \frac{q_i q_j}{r_{ij}} (9 \times 10^9) \text{ Joules}$$

for q in coulombs
r_{ij} in meters.

= **1328 kJ/mol** per $\frac{e^2}{A^\circ}$

Atoms are treated as point charges and point masses.

Some typical values:

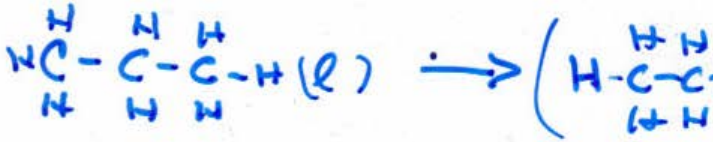


Hydrogen bonding is almost all electrostatic attraction of partial charges. It is strong because of ***smallness of H;***

H gets closer than any other atom!

HYDROPHOBIC "INTERACTIONS"

OIL & WATER DON'T MIX

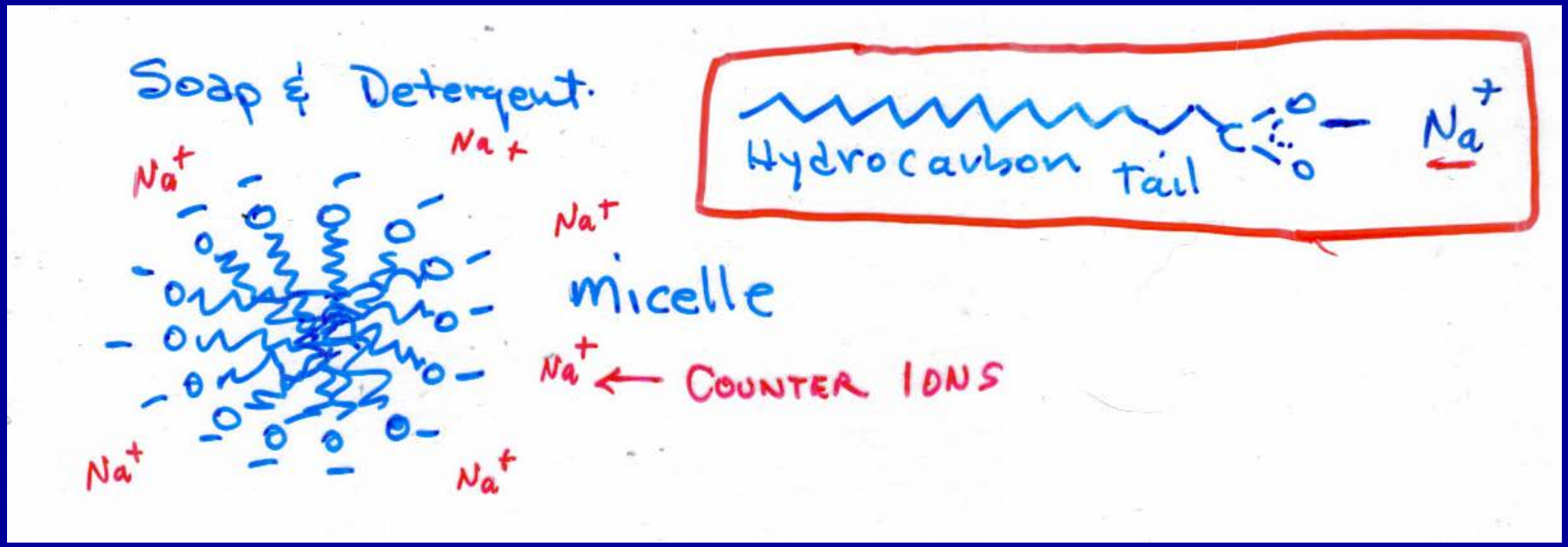


$\Delta H^\circ = -8$ kJ/mol

$\Delta S^\circ = -80 \frac{J}{mol\ K}$

$$\Delta G^\circ = \Delta H^\circ - 298(\Delta S^\circ) = +16 \text{ kJ/mol.}$$

- Water ORDERS around the hydrocarbon
- heat given off as in freezing of water.


Soap & Detergent.
Hydrocarbon tail
Na+
Na+
Na+
Na+
Na+
Na+
Na+
micelle
Na+ ← COUNTER IONS

BIOLOGICAL SOAPS ≡ LIPIDS ≡ FATS.

FORM BILAYERS ≡ MEMBRANES.

AND VESICLES

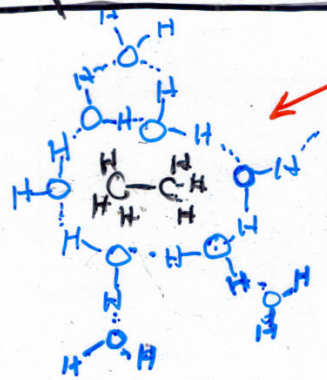
(for transporting.)

e.g. neutral transmitters)

Hydrophobic "Interaction"

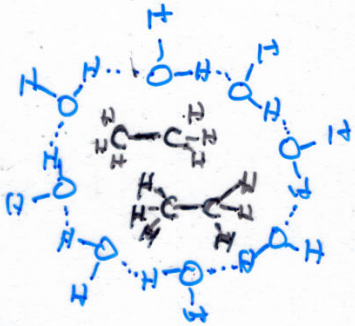
separate ethanes

2



2 × 6 = 12 ordered H_2Os

→



but only 8 ordered waters if the 2 ethanes are adjacent.

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.

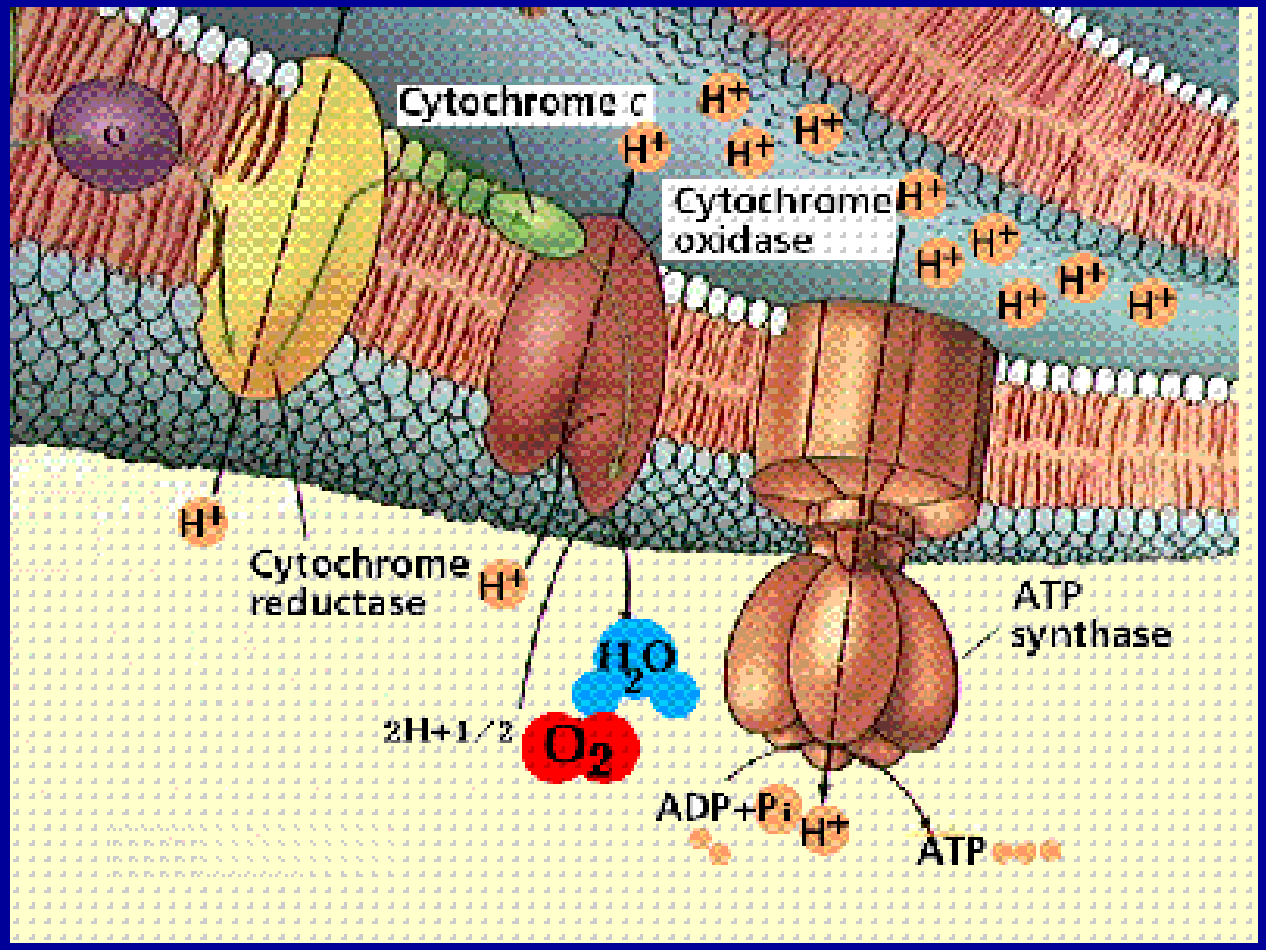
What are proteins and what do they do?

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.


Cytochrome c
Cytochrome oxidase
Cytochrome reductase
ATP synthase
H^+
H_2O
$2H+1/2$
O_2
ADP+Pi
ATP

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

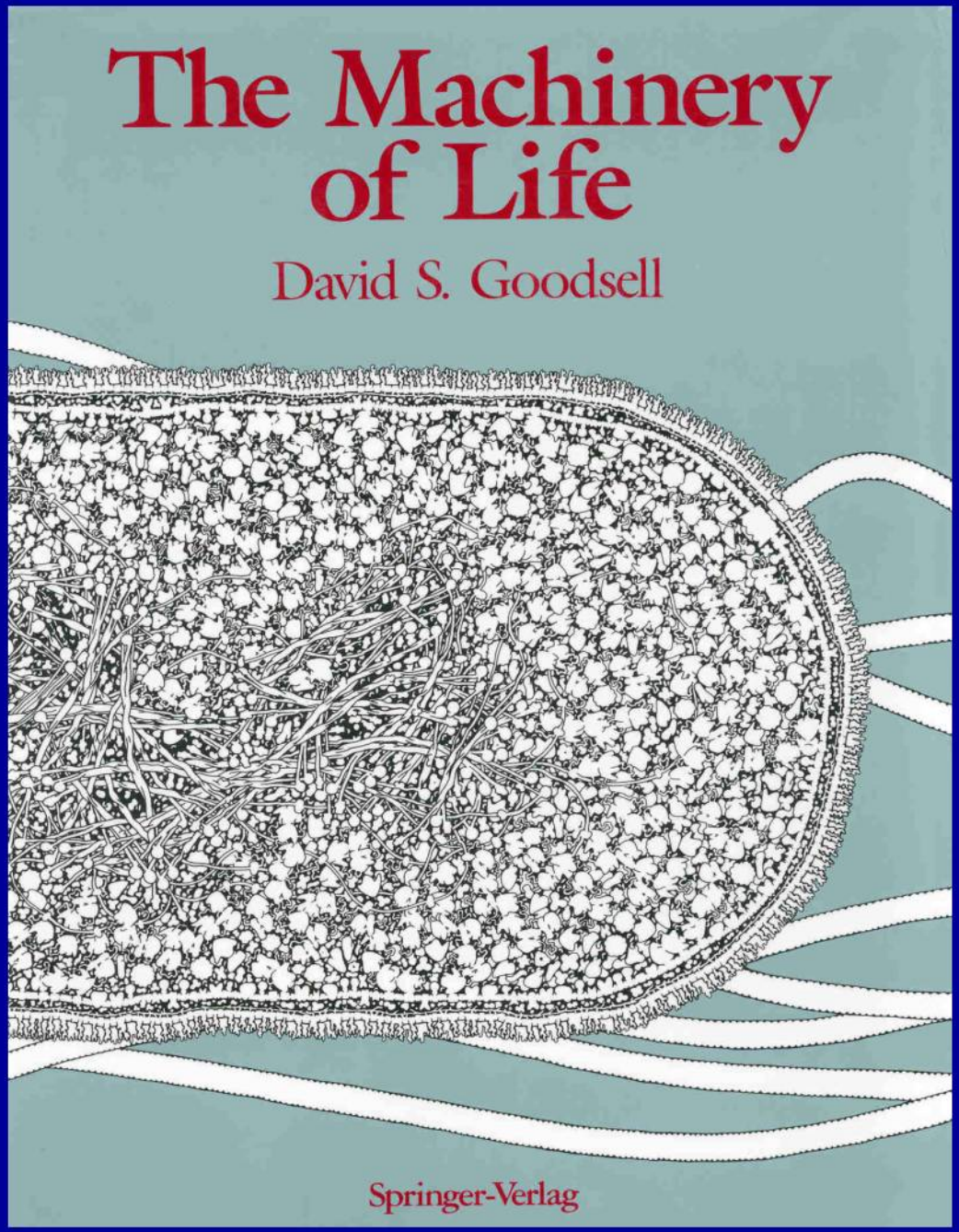
Immune protection

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.



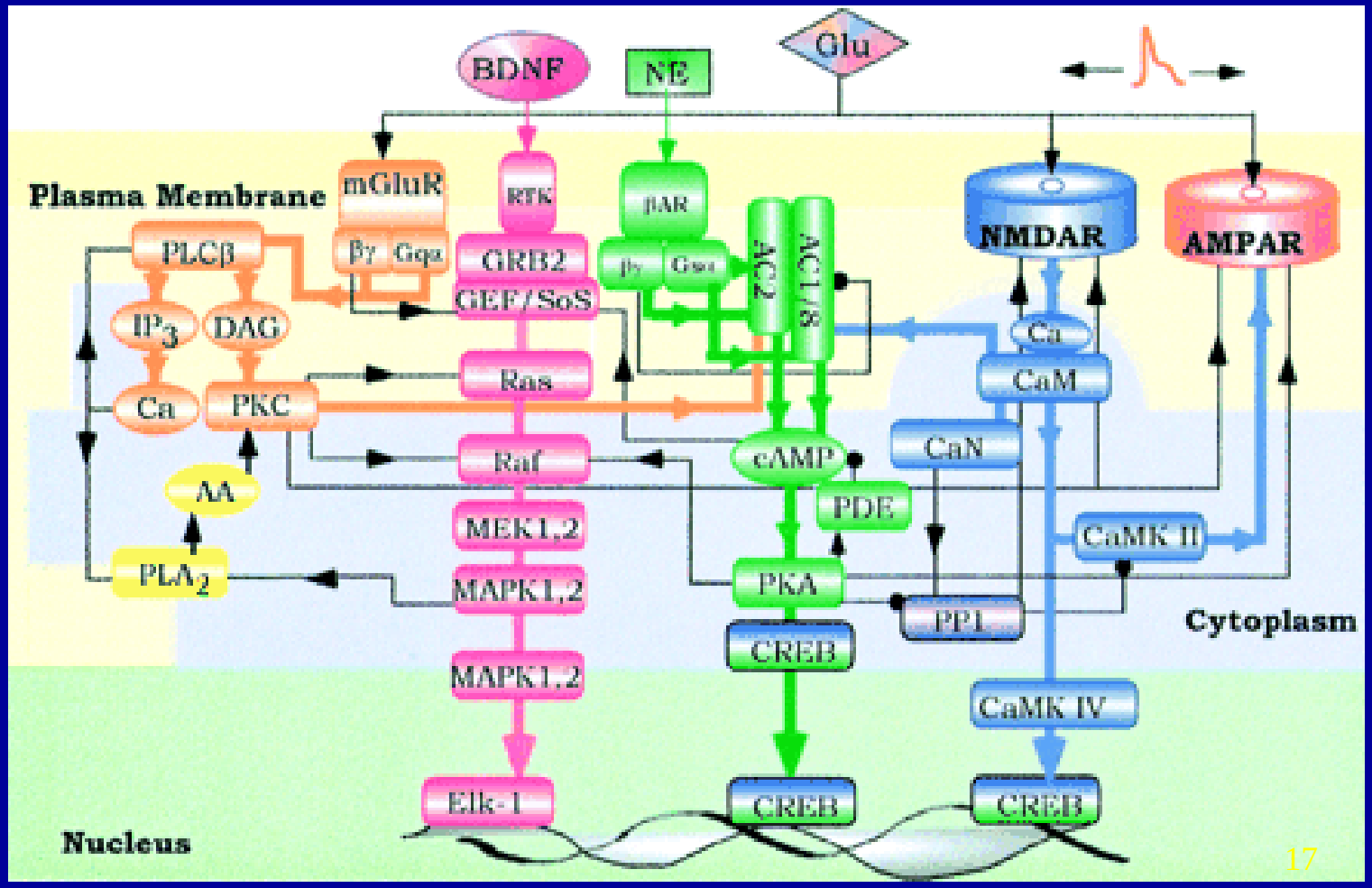
The visual answer

Ecoli Bacterium

Interacting Signaling Pathways

= ligands

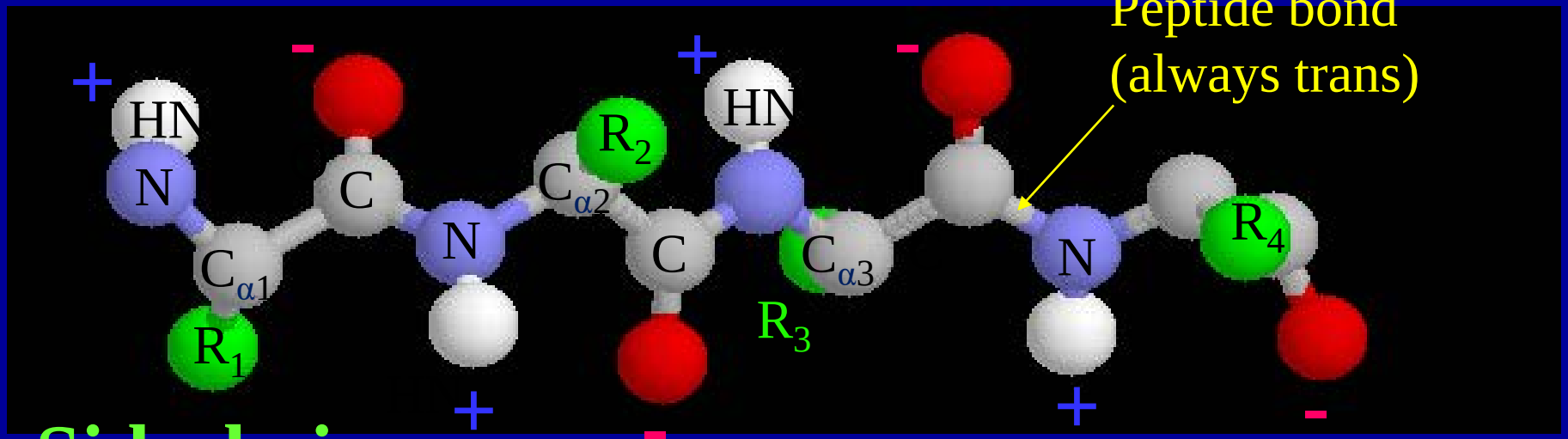
= PROTEINS



What are proteins? **The chemical answer:**

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

Backbone



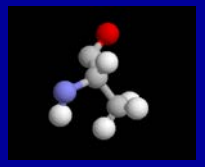
Sidechains

H on each C_α not shown

Tiny

Gly

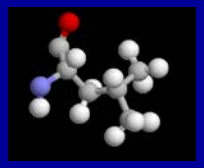
Ala



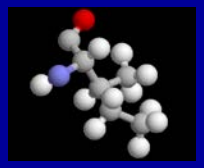
Oil and Gasoline

Val

Leu

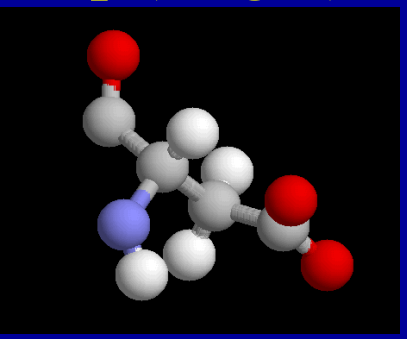


Ile

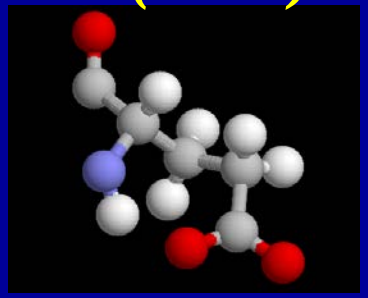


Negatively Charged

Asp *(vingar)*

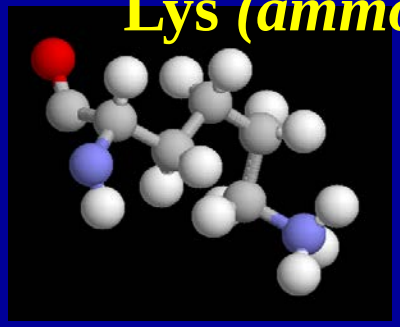


Glu *(MSG)*

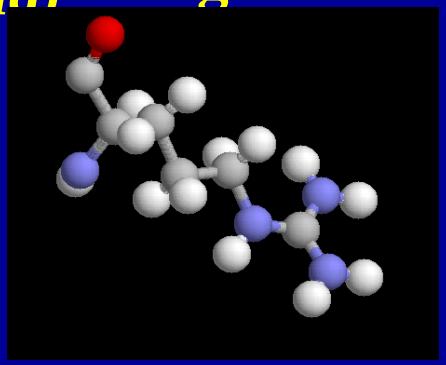


Positively Charged

Lys *(ammonia)*

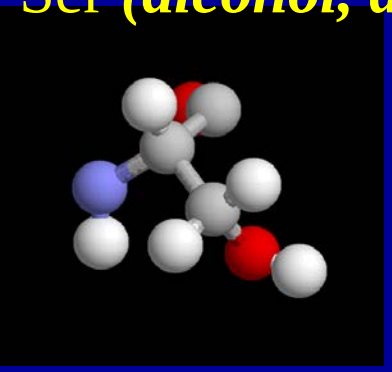


Arg

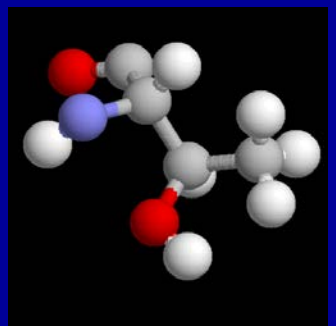


Polar , uncharged

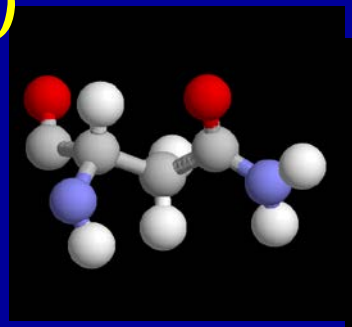
Ser ***(alcohol, drinking)***



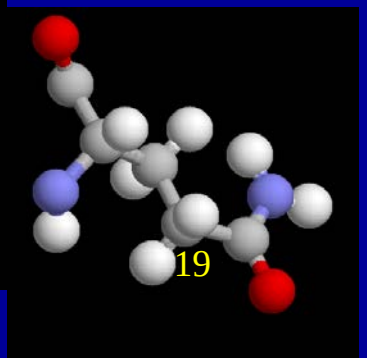
Thr ***alcohol, rubbing)***



Asn

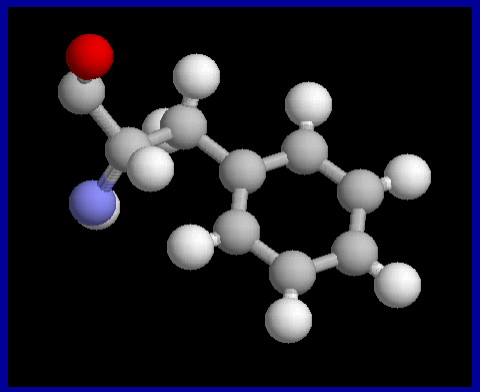


Gln

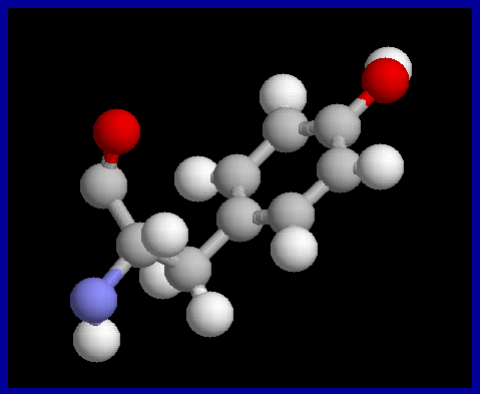


Aromatic Hydrophobic *(UV absorbing)*

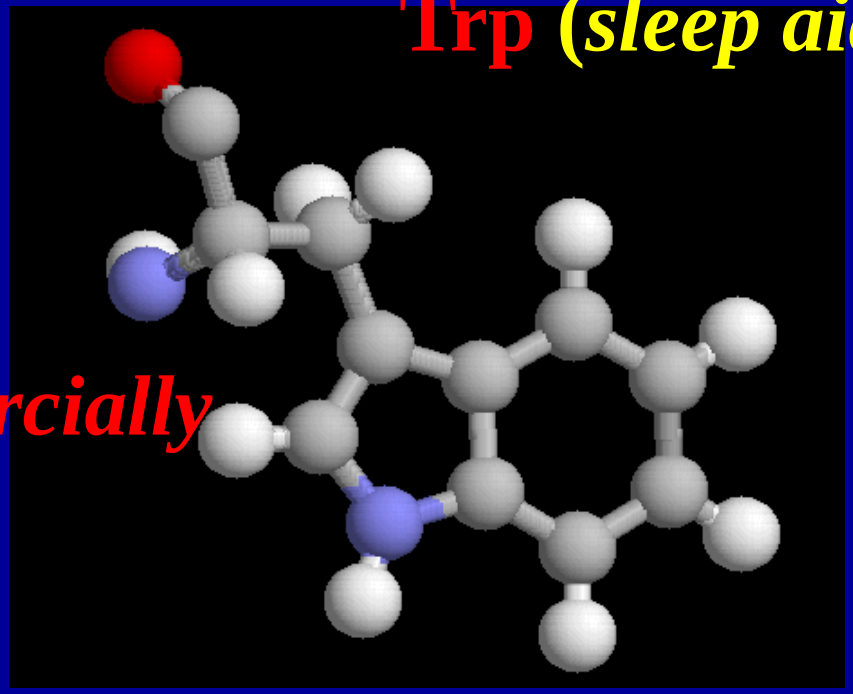
Phenylalanine
(benzene)



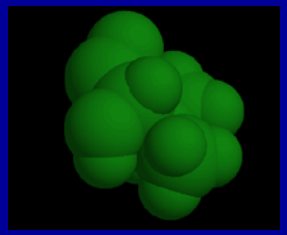
Tyrosine (*phenol*)



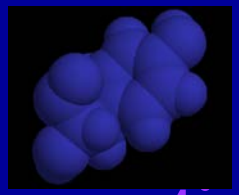
Tryptophan
Trp (*sleep aid*)



Banned. Cannot
be made safe commercially
Really???

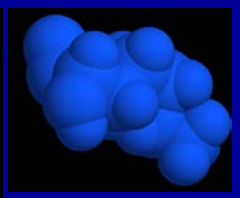


Aliphatic

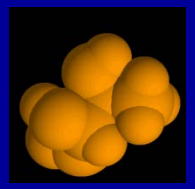


Aromatic

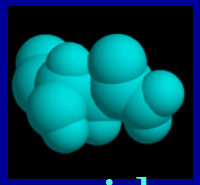
Neg



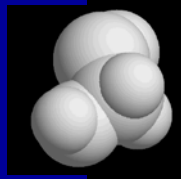
Pos



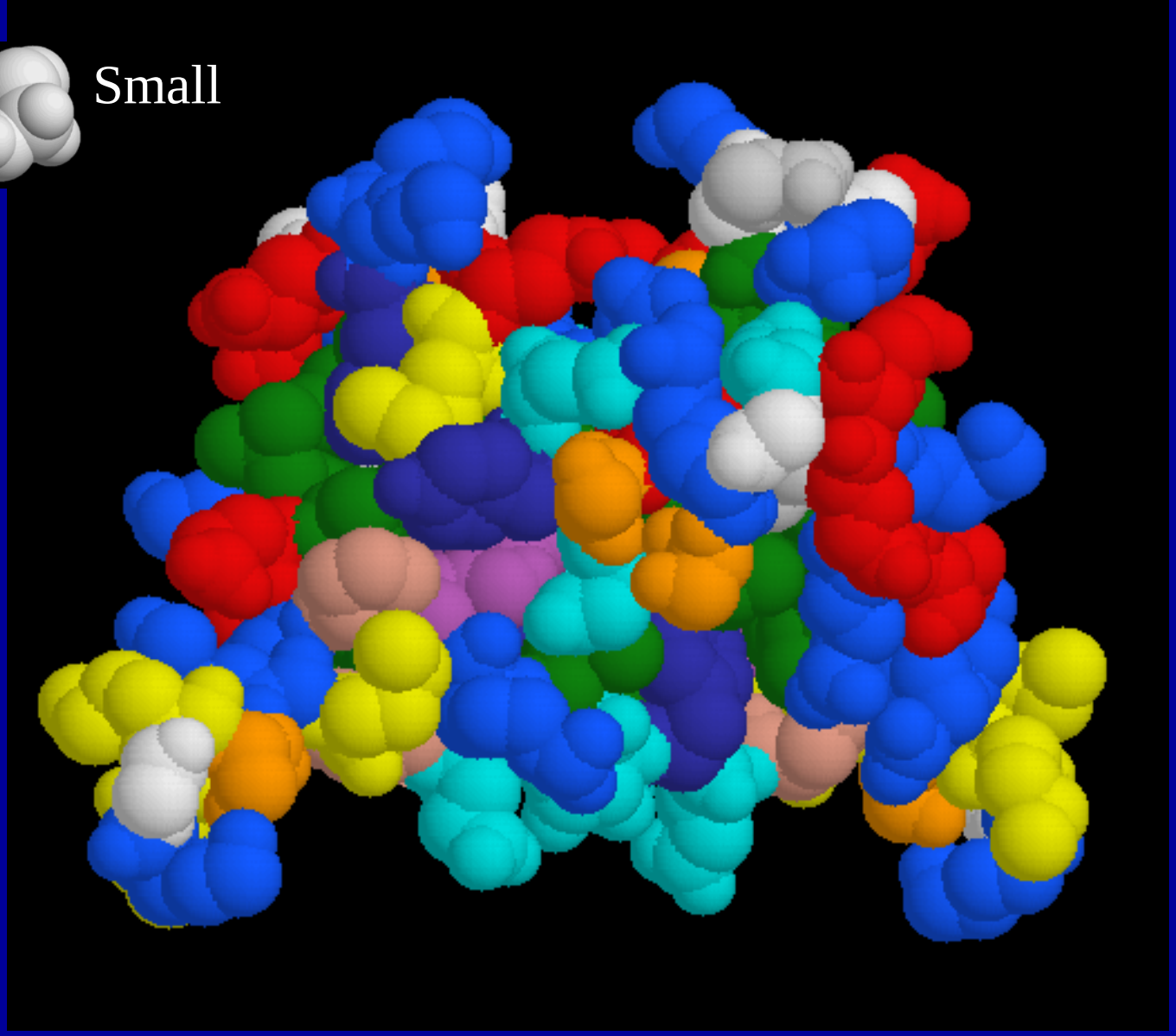
alcohol



amide



Small



Methionine