Cells are mostly made of the most abundant chemical elements, H, C, O, N, Ca, Mg, Na, K, P, etc.

The strongest bond between atoms is the covalent bond. The C-C bond is about 90 kcal/mol $\simeq$ 3.9 eV

$$1 \text{ kcal/mol} \simeq 0.04336 \text{ eV}$$

$$1 \text{ mol} = 6.022 \times 10^{23} \text{ molecules}$$

$$= 4.0026 \text{ g of He, for example.}$$

The H_2 molecule is held together by a single covalent bond

$$H = H_0 + V$$

$$H_0 = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} - \frac{e^2}{|r_1 - R_1|} - \frac{e^2}{|r_2 - R_2|}$$

$$V = \frac{e^2}{|\vec{R}_2 - \vec{R}_1|} + \frac{e^2}{|R_2 + r_2 - R_1 - r_1|} - \frac{e^2}{|R_2 + r_2 - R_1|} - \frac{e^2}{|R_2 - R_1 - r_1|}.$$

H is invariant under the interchange of r_1 with r_2. So its e-states may be chosen to be e-states of the operator, T, that exchanges the electrons.

Since electrons are fermions, their e-states must be antisymmetric under exchange of two electrons.

H does not involve spin to this order. So we may choose the spin state to be symmetric or antisymmetric.
$S = 1$ $\qquad\qquad\qquad$ $S = 0$.

The space state then would be antisymmetric or symmetric, respectively.

Which?

In fact the space state is <u>symmetric</u> and the spin is zero. The two electrons clump together and so attract the two protons. The binding energy $V(r)$ is a function of the separation

$$r = |R_2 - R_1|$$

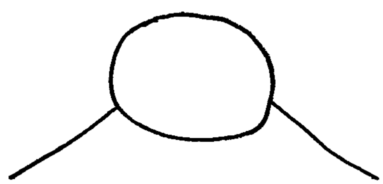
at $r \simeq 0.74 \mathring{A}$, $\quad V(r) \approx -4.75 eV$
$\simeq -110$ kcal/mol.

A useful parametrization of $V(r)$ is

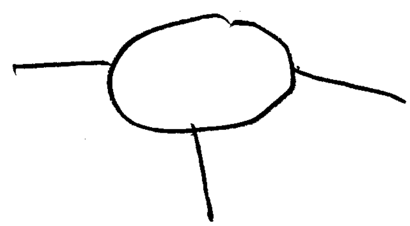
$$V(r) = a e^{-br}(1 - cr) - \frac{d}{r^6 + e r^{-6}} .$$

The fit is very good.

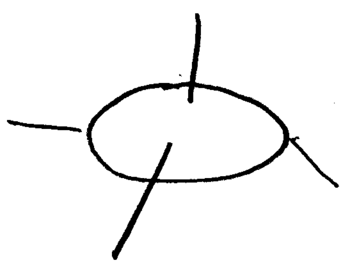
Some atoms have more than one covalent bond



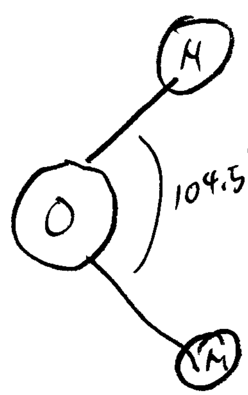
O



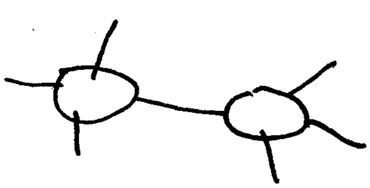
N



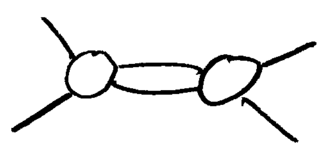
C



water



ethane

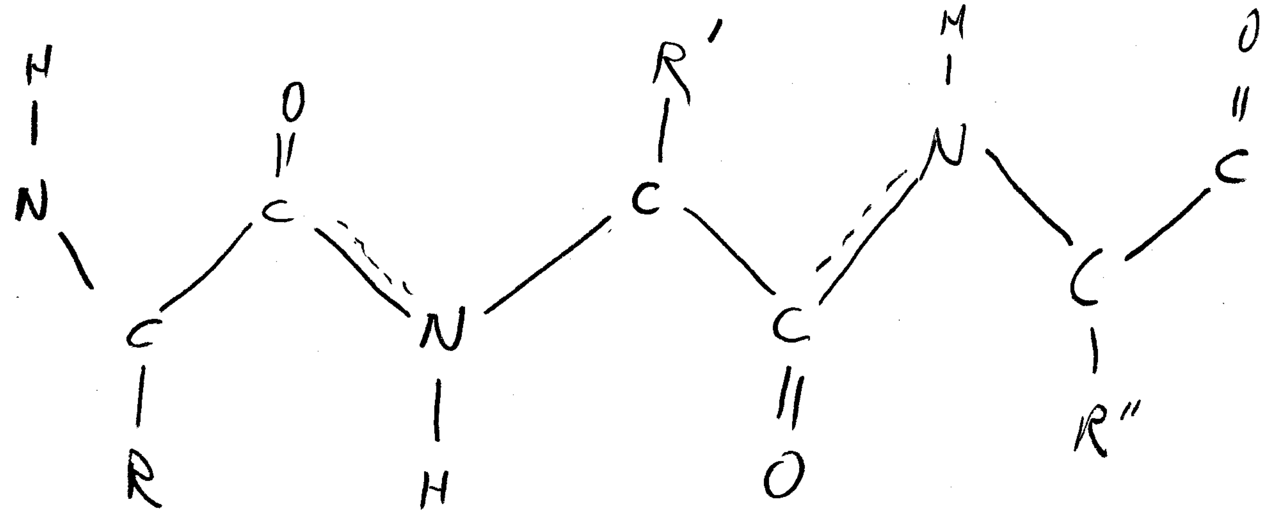


ethene, planar

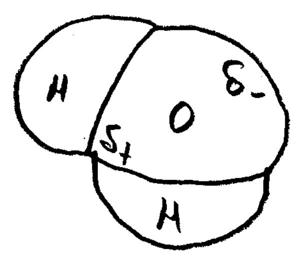
Single bonds allow rotations.

Double, triple bonds do not.

Some bonds are in between single and double bonds, e.g., the peptide bond C–N is a 1.5 bond, and it resists rotation.



Water, H_2O, is the most abundant molecule in cells.

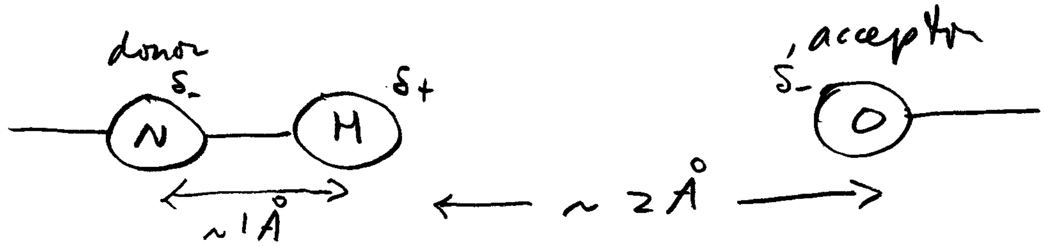


Water has a large permanent electric dipole moment.

Non-covalent bonds:

1) Ionic bonds, e.g., NaCl = $Na^+ Cl^-$. Is this a covalent bond in which the electrons clump on the Cl atom?

2) Hydrogen bonds



directional

3) van der Waals: How very light electrons respond to the array of charges near them. At a few Å,

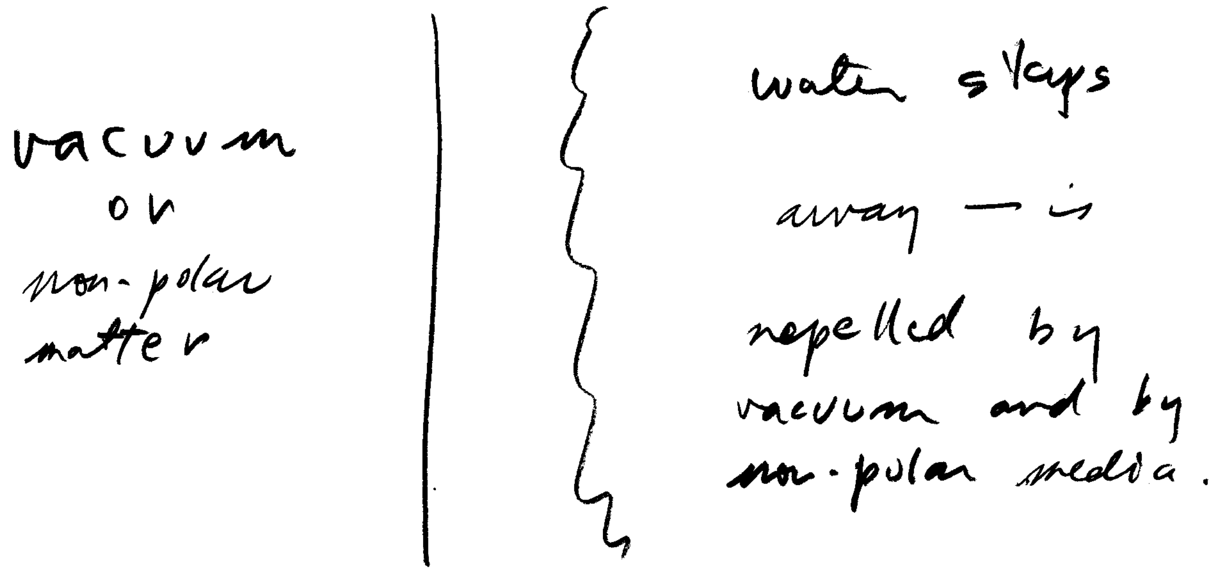
$$V(r) \sim -\frac{d}{r^6}$$

at longer distances

$$V(r) \sim -\frac{e}{r^7}.$$

4) hydrophobic force: polar water molecules

are attracted to each other and to other polar molecules.



bond	length (Å)	E (vac)	E (H_2O
covalent	1.5	90	90
ionic	2.5	80	3
H	3	4	1
vdW	3.5	.1	.1

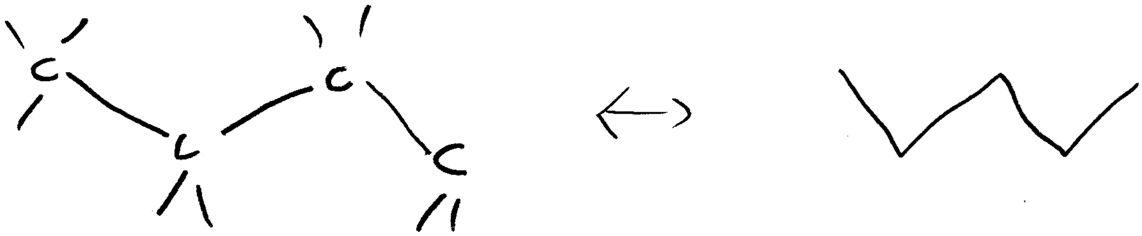
kcal / mol.

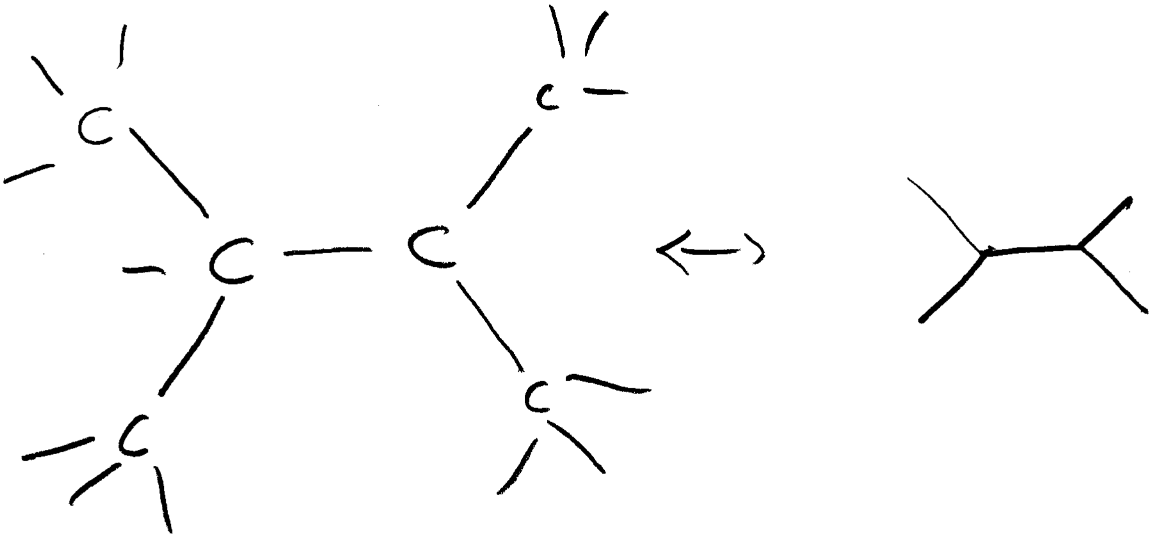
examples of H bonds

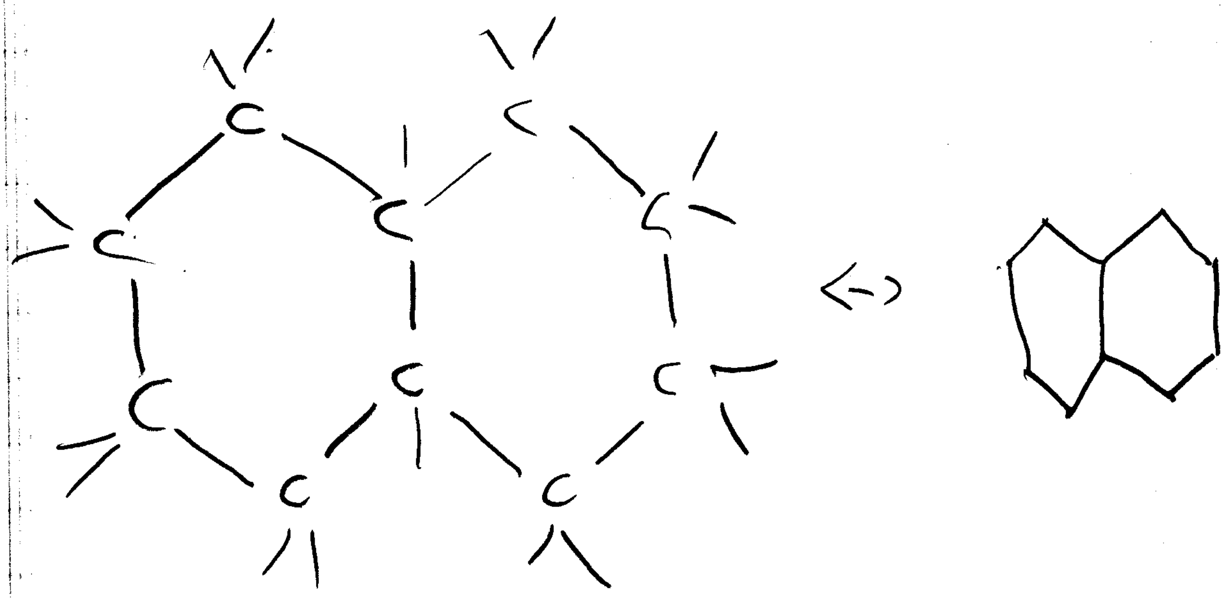
N - H	O
O - H	O^-
O - H	N
N^+ - H	O
N - H	N

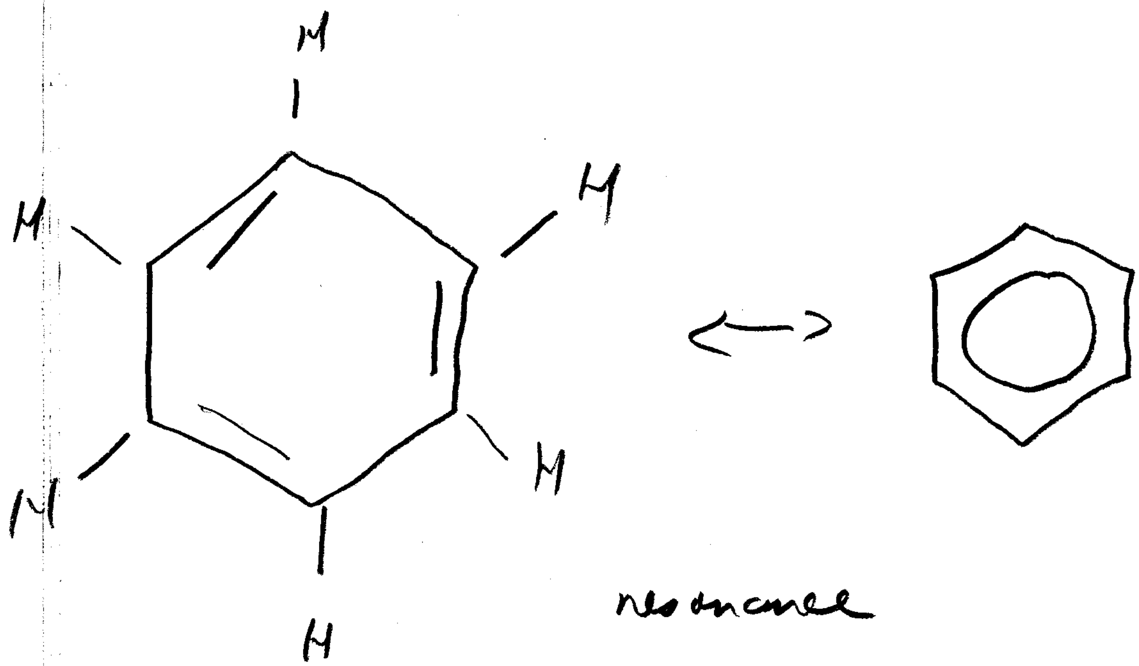
Bacterial cell has

		# kinds
Water	70%	1
inorganic ions	1	20
sugars	1	250
amino acids	.4	100
nucleotides	.4	100
fatty acids	1	50
small molecules	.2	~300
big "	26	~3000

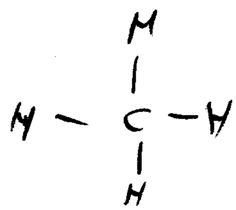




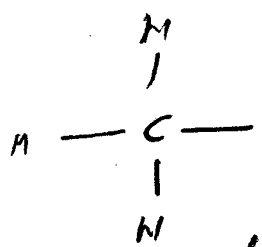




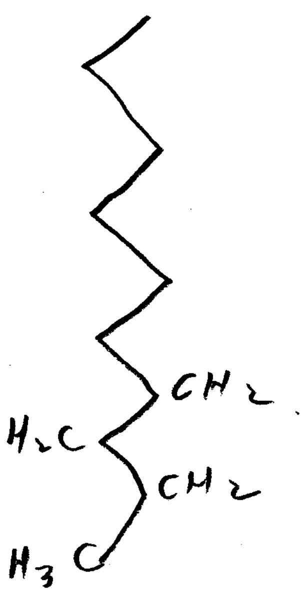
resonance



methane



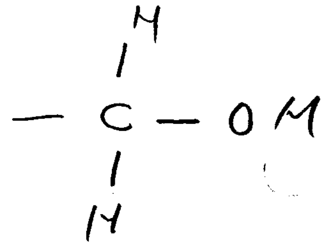
methyl group



saturated
hydrocarbon

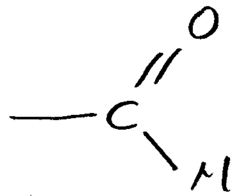
C-O groups

alcohol



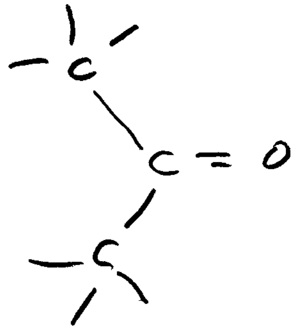
$-OH$ hydroxyl

aldehyde

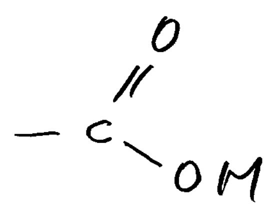


$C=O$ carbonyl

ketone



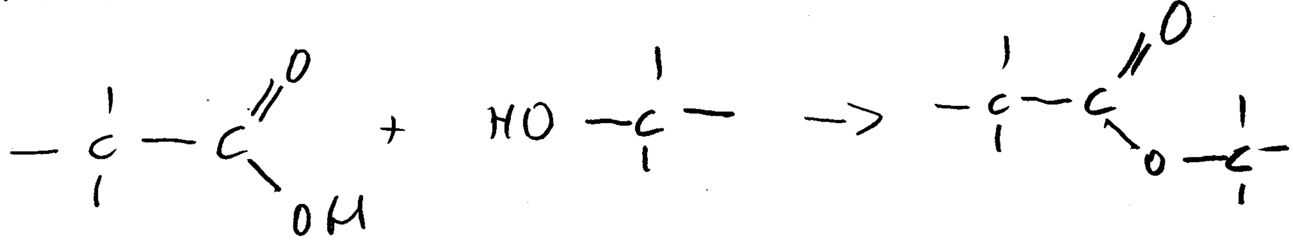
carboxylic acid



$$-COO^- + H^+ \leftarrow -COOH$$

in water — carboxyl group

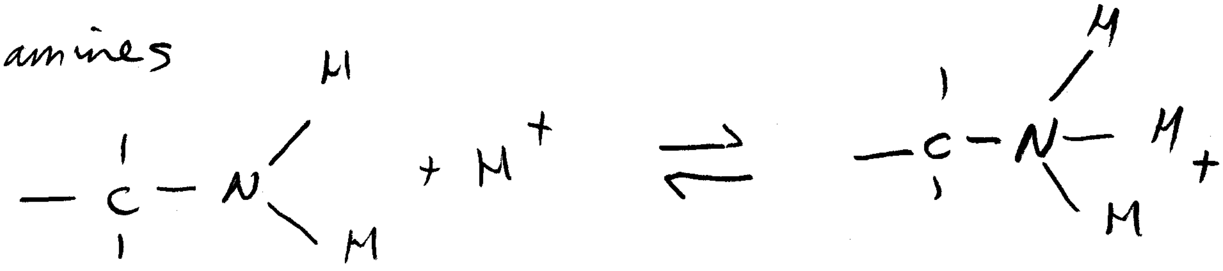
esters



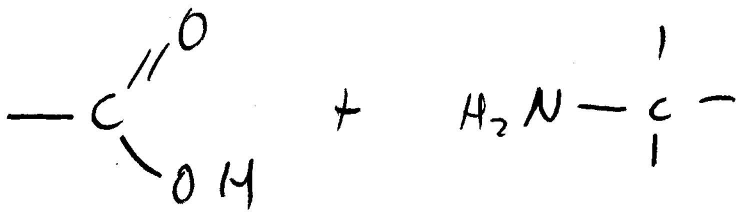
acid — alcohol — $+ H_2O$

C-N groups

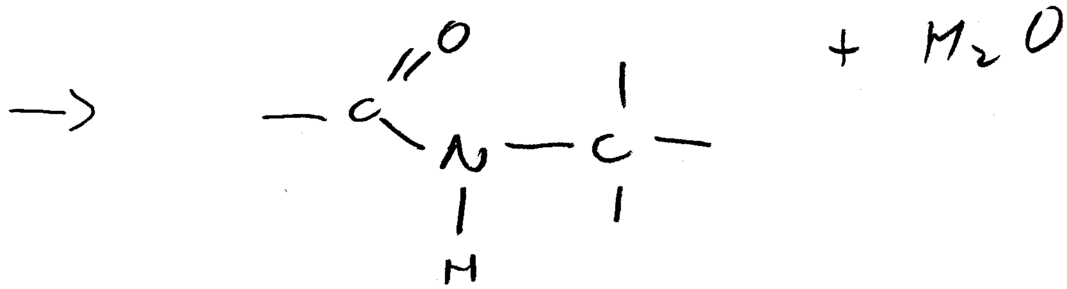
amines



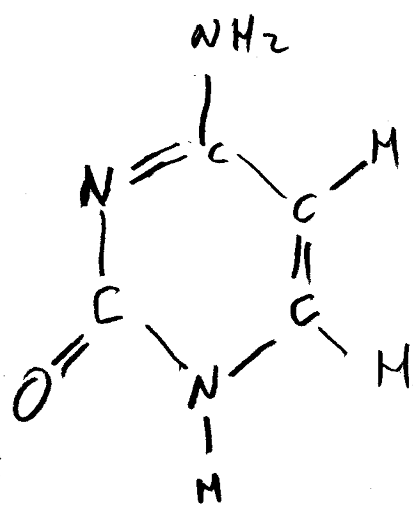
amides



acid amine

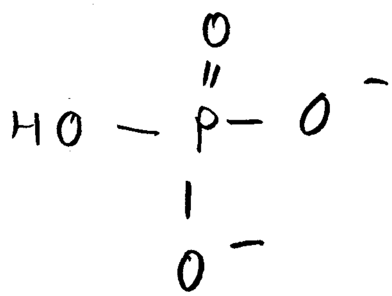


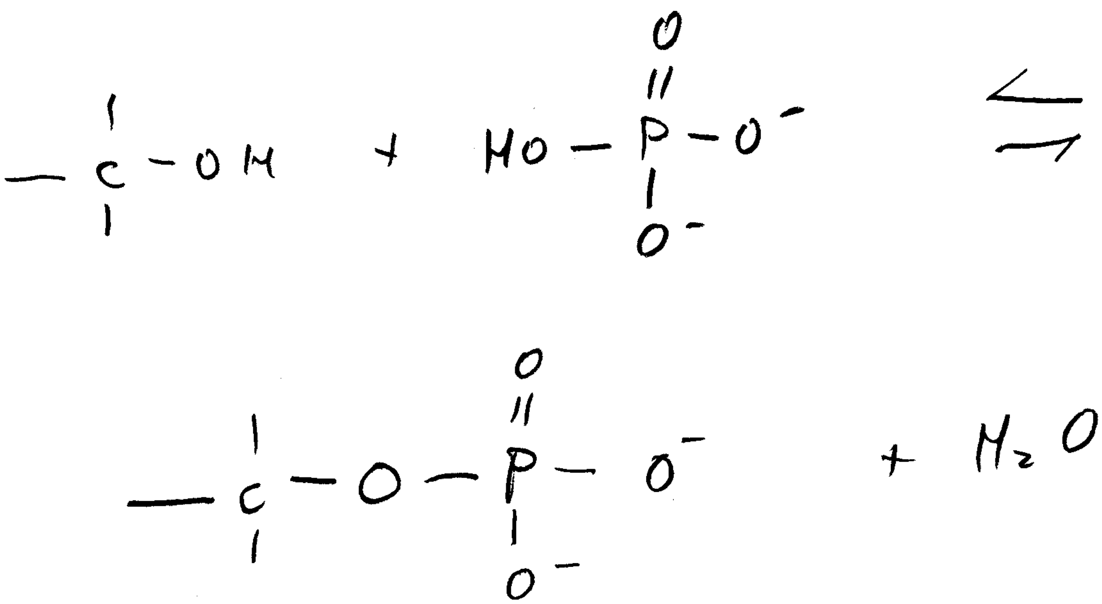
amide (uncharged in H_2O)



cytosine a pyrimidine

phosphates





phosphate ester