Organic chemistry

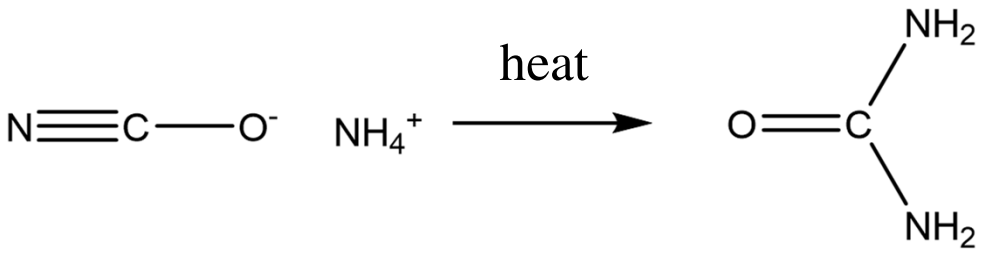
MARTIN VEJRAŽKA

Organic chemistry

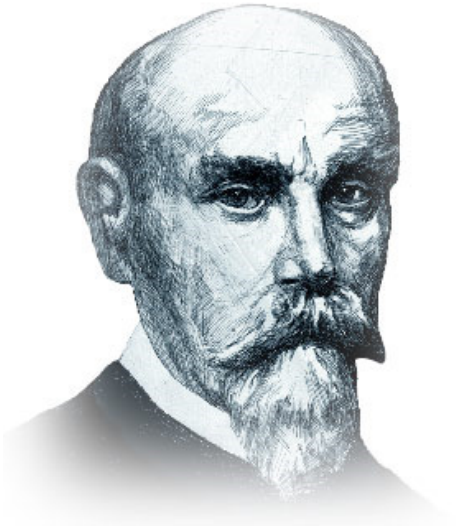
Fridrich Wöhler

1800-1882

Synthesis of urea from ammonium cyanate (1828)



Jan Horbaczewski



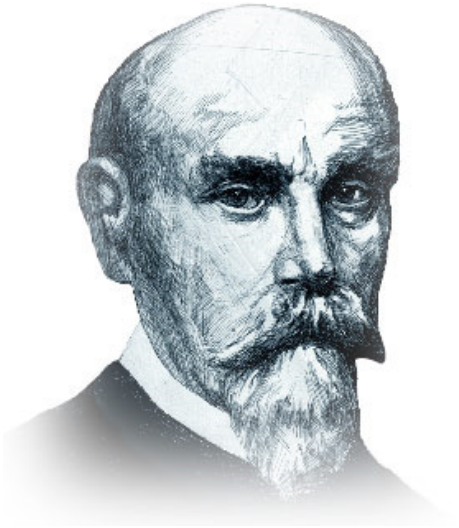
1854-1942

Absolved medical school of Vienna

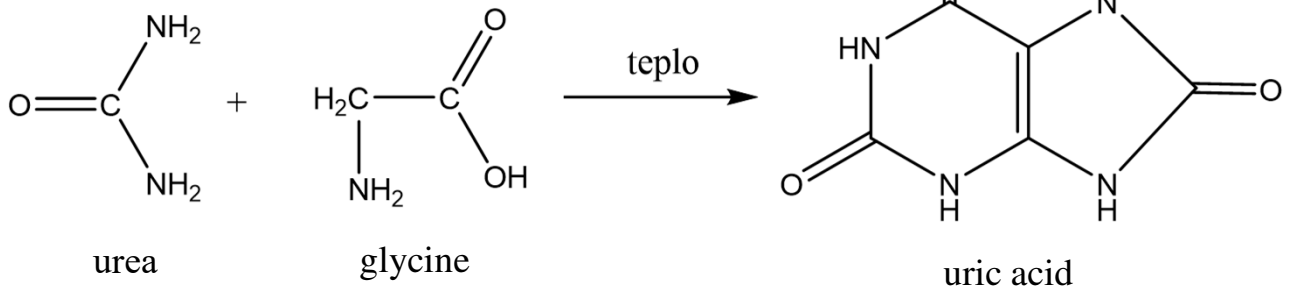
Founded Institute of Medical Chemistry (1883)

Synthetised uric acid (1882)

Jan Horbaczewski

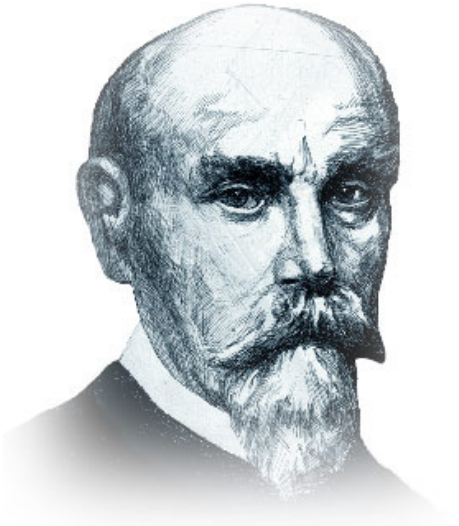


1854-1942



urea glycine uric acid

Jan Horbaczewski

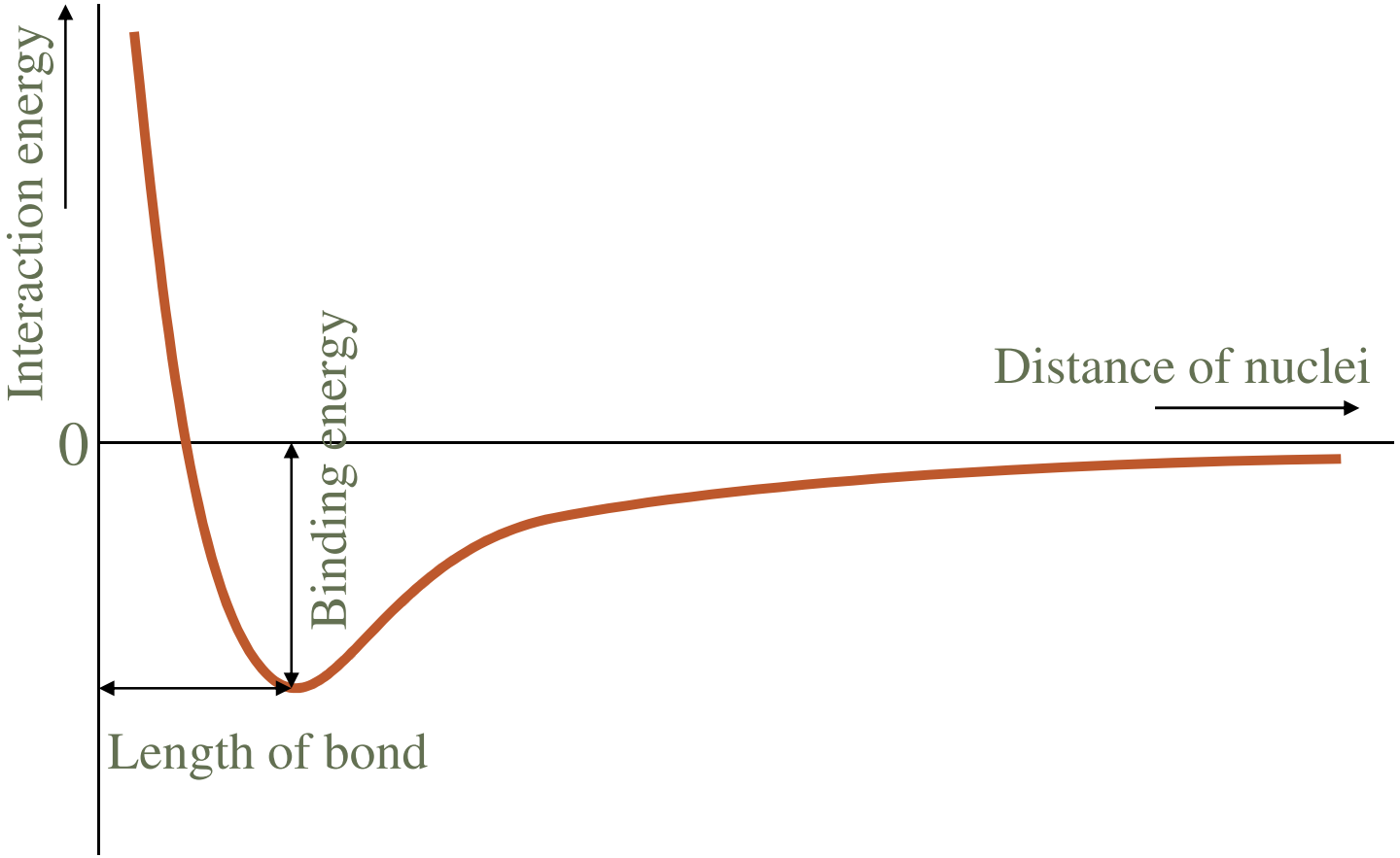


1854-1942

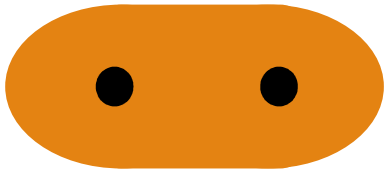
Further experiments:

- Uric acid raises from degradation of cells with **nucleus** only
- **Separated** uric acid from **xanthine** and other **purines**
- Predicted that uric acid is degradation product of them

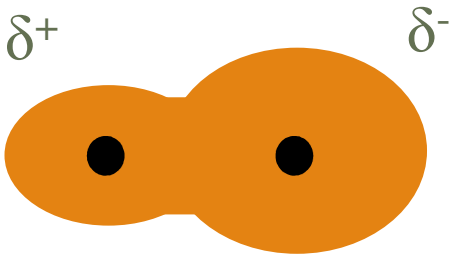
Bonds in organic compounds


Interaction energy
0
Binding energy
Distance of nuclei
Length of bond

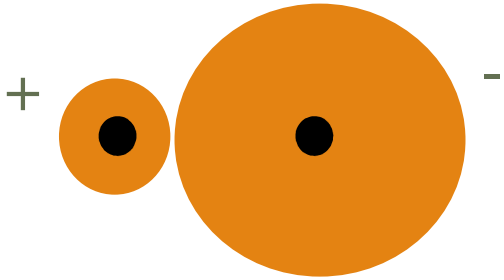
Chemical bond



Non-polar



Polar

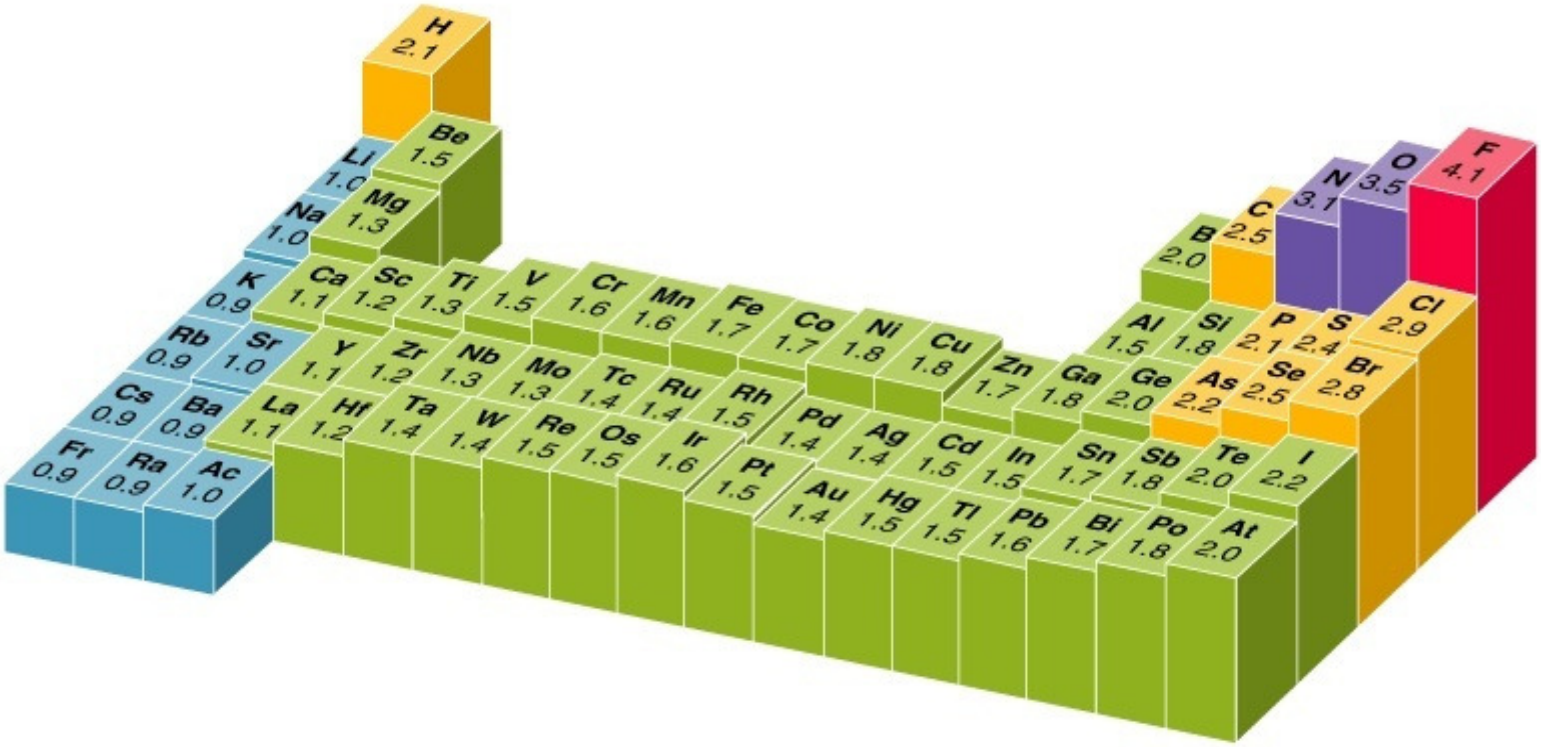


Ionic

Polarity of bond

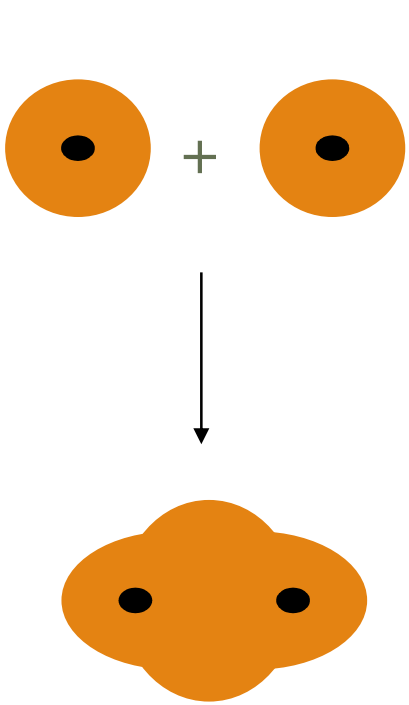
	Difference in electronegativity
Non-polar	< 0.4
Polar	0.4–1.7
Ionic	> 1.7

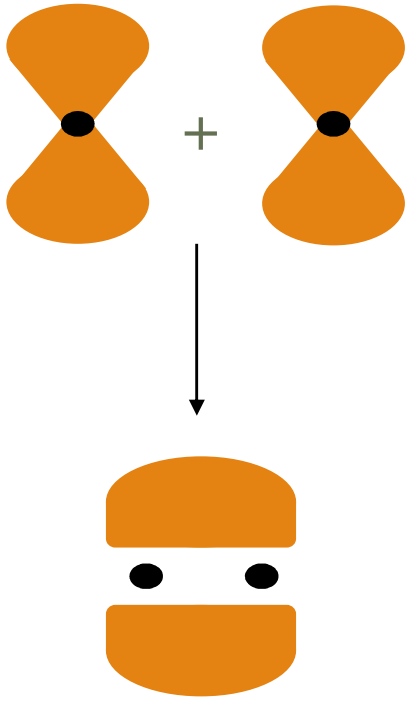
Electronegativity



https://www.quora.com/What-are-the-definitions-of-oxidation-number-and-formal-charge

σ and π





Covalent bond

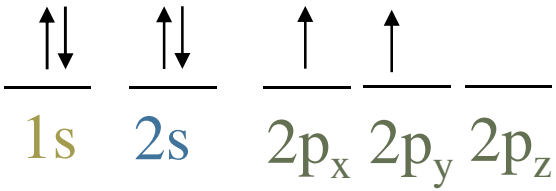
σ	π
Longer	Shorter
Can rotate	Cannot rotate

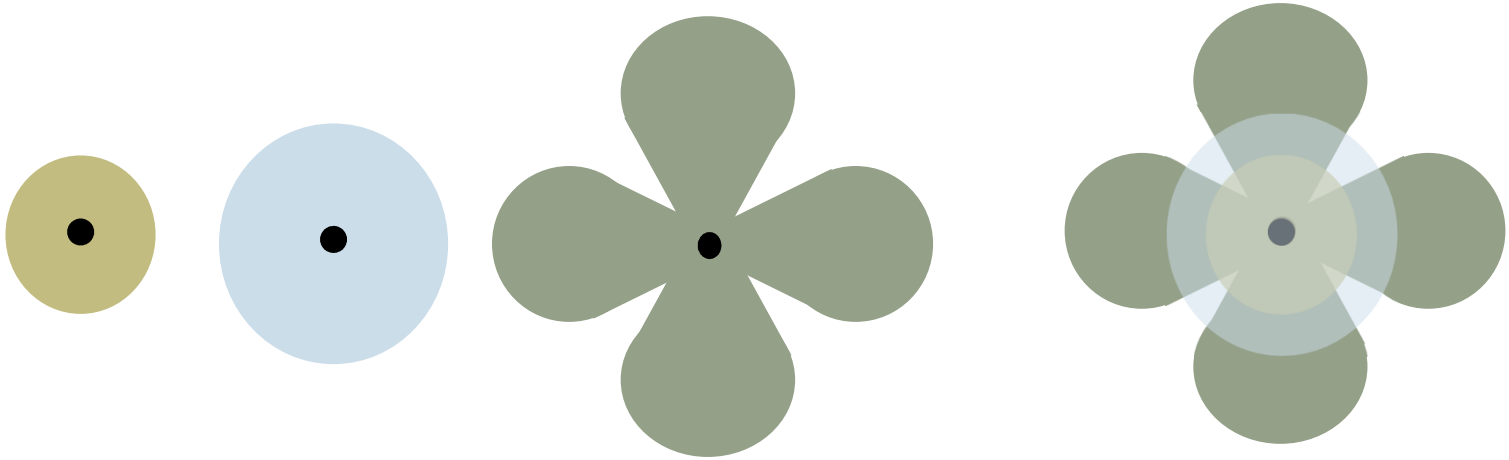
Multiple bond
stronger

Orbital hybridization

Ground electron configuration of carbon C

$1s^2\ 2s^2\ 2p^2$

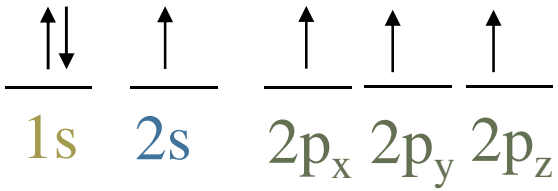


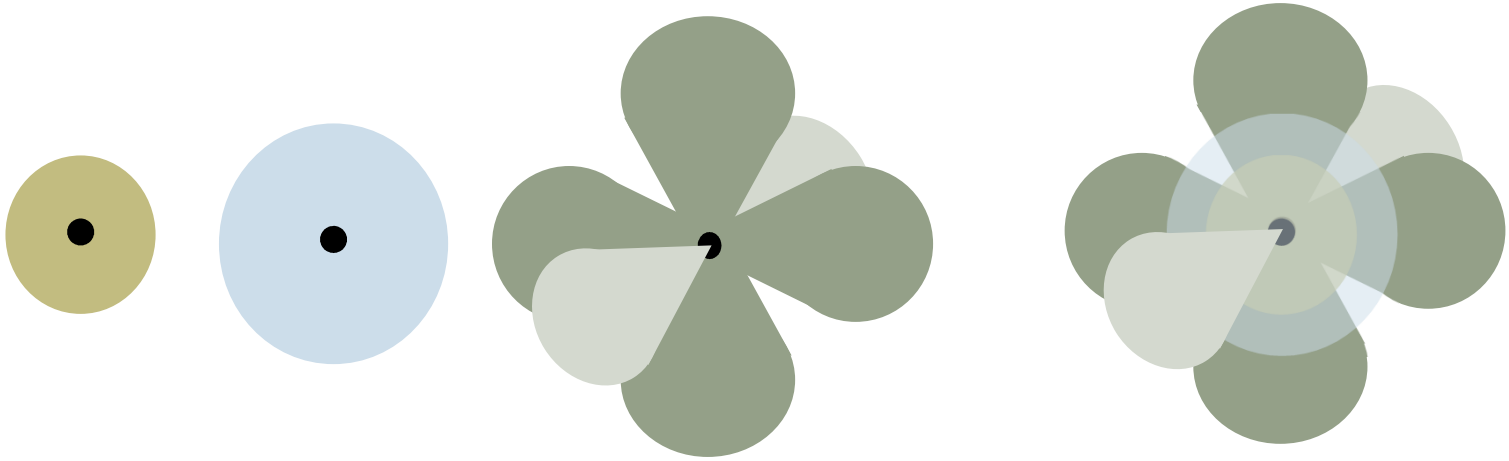


Orbital hybridization

Excited state C^*

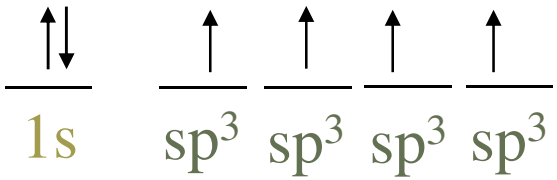
$1s^2\ 2s^1\ 2p^3$

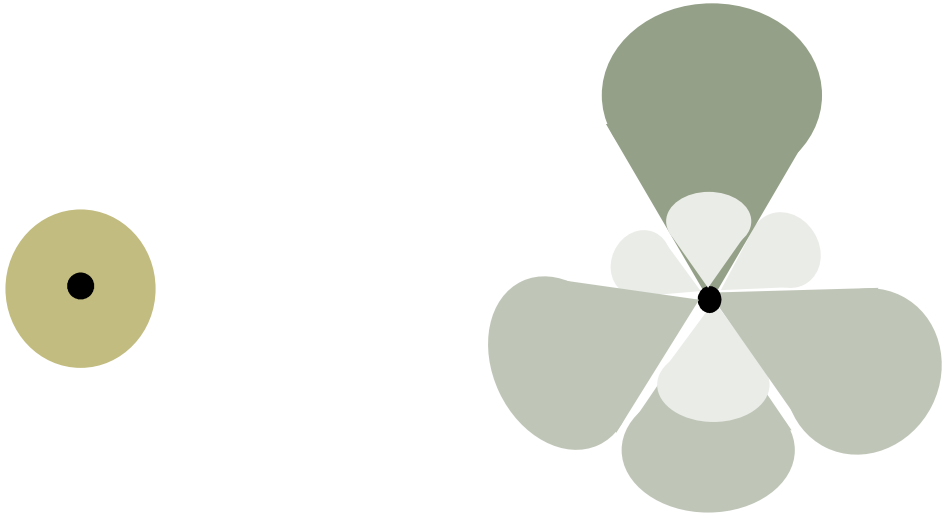




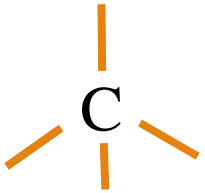
Orbital hybridization

Hybridization C*

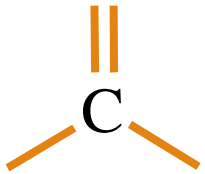




Orbital hybridization

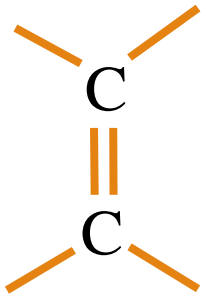


sp^3



sp^2

sp



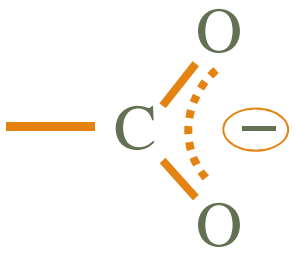
Cannot rotate!

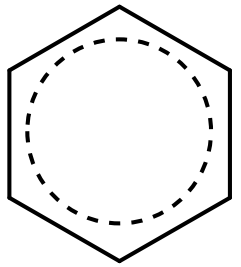
Hybrid bonds

E.G. „1.5×“ bond

- Longer than double, shorter than single
- Energetic properties between single and double
- Cannot rotate

- Carboxylic group
- Benzene nucleus





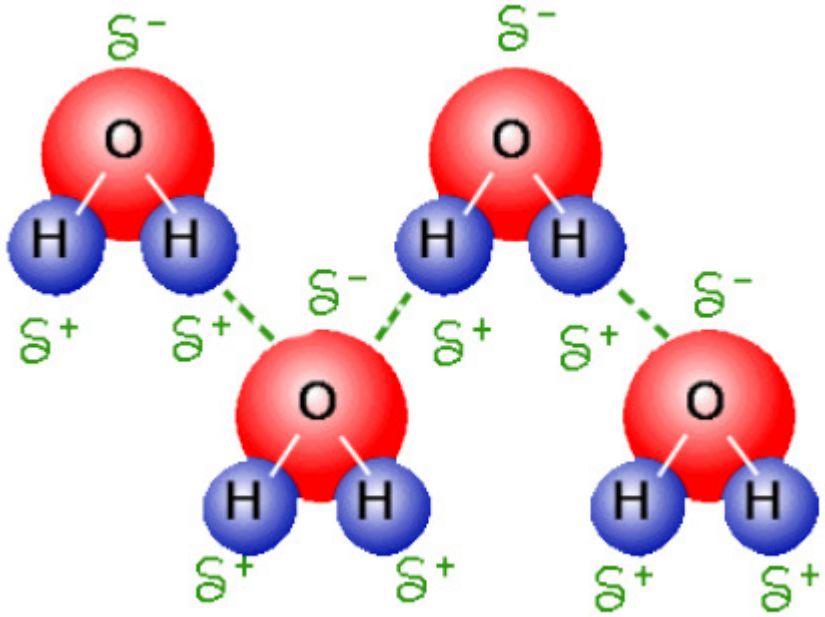
Non-bonded interactions

- Van der Waals force
  - Mostly in non-polar compounds
- Hydrophobic interactions

https://www.flickr.com/photos/lizard_queen/97118836

Non-bonded interactions

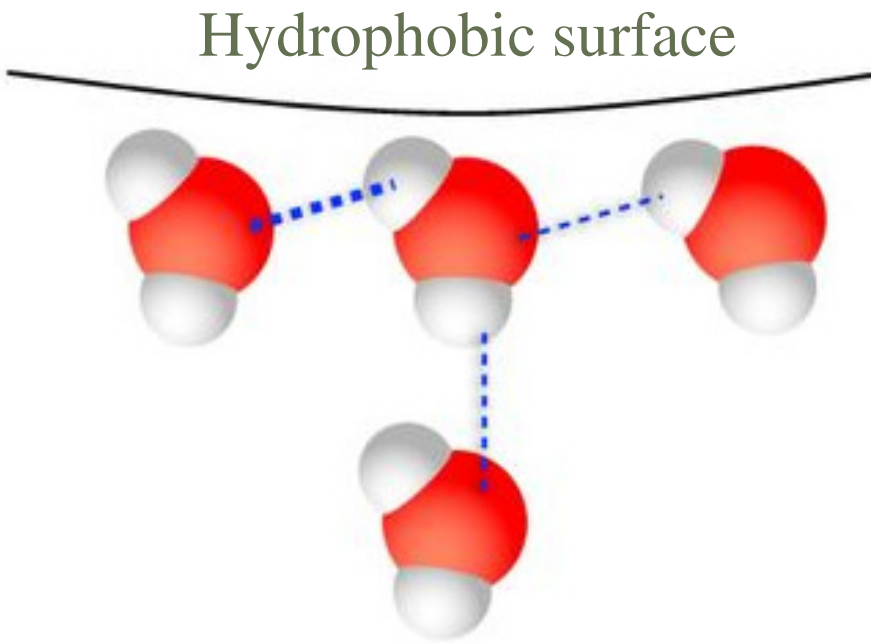
Hydrogen bridges



10× weaker than ionic and covalent bonds

Non-bonded interactions

Hydrophobic interaction



http://rsif.royalsocietypublishing.org/content/10/79/20120835

Organic molecules

Organic formulas

Summation formula

Structural formula

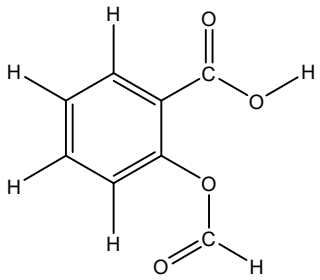
- All bonds
- Confusing

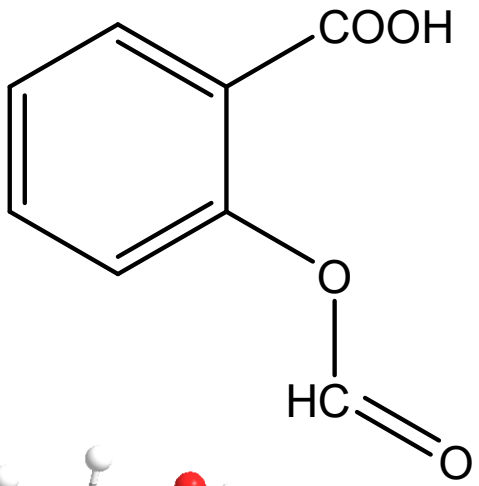
Rational

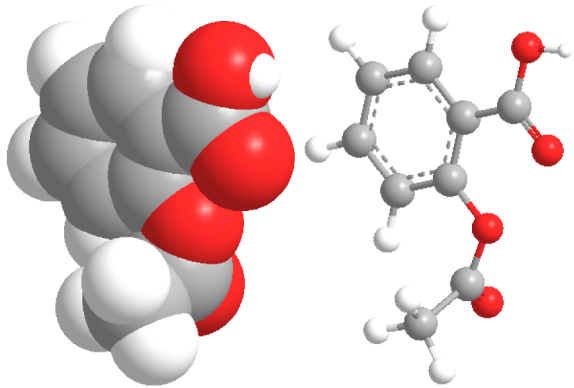
- Most used

Perspective

- Arrangement in space







Isomerism and conformation

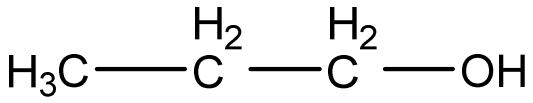
Isomers: Identic summation formula, different arrangement

Isomeration = breaking and making bonds

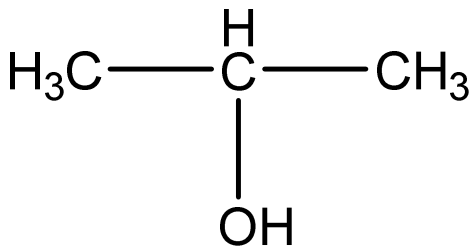
Conformers: Various arrangement in space – rotation around bonds

Change of conformation – no breaking and making bonds

Constitutional isomers

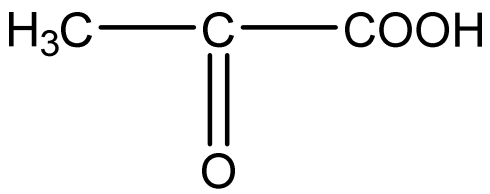


1-propanol

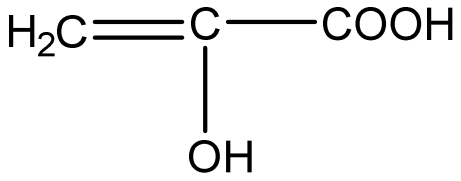


2-propanol

Tautomers



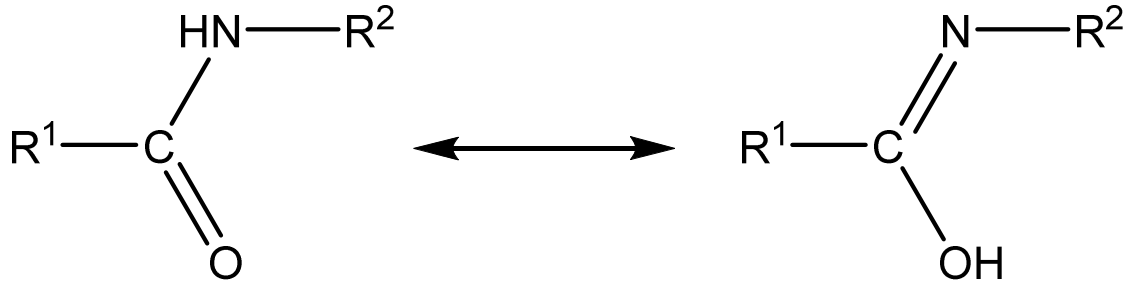
Keto-form



Enol-form

Tautomers are isomers
but they mostly can change each into the other spontaneously

Peptide bond



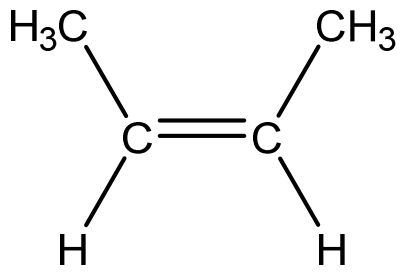
Keto-form

Enol-form

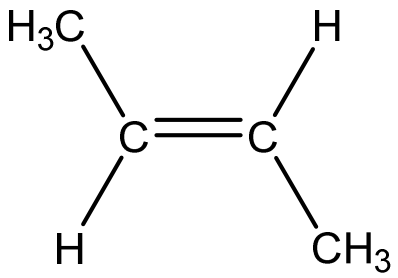
Properties of „1.5×“ bond

- Shorter than single
- Cannot rotate

Configuration isomerism

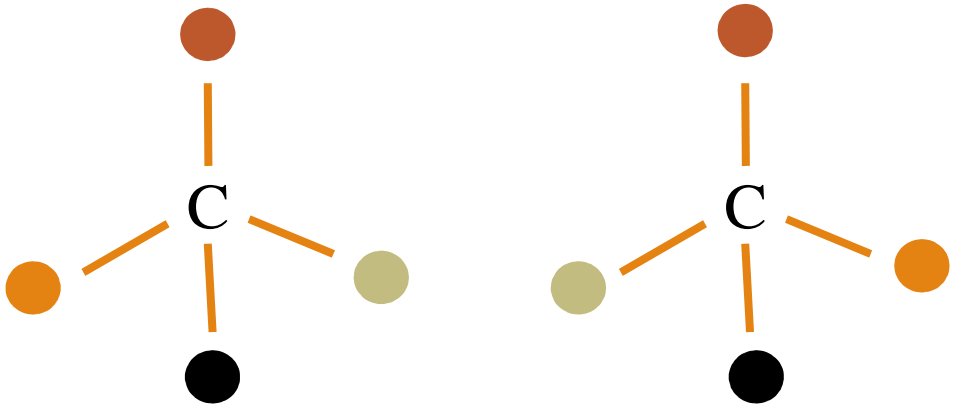


cis-buten



trans-buten

Optical isomerism



Compounds with center of chirality are optically active

Selected derivatives of hydrocarbons

Halogen derivatives

Bonds C-Cl, C-Br, C-I are **non-polar**

- Mostly non-polar **solvents**, volatile
- E.g. tetrachlormethane CCl_4, chloroform CCl_3H
  - Narcotics
- **Freons** (e.g. CCl_3F)

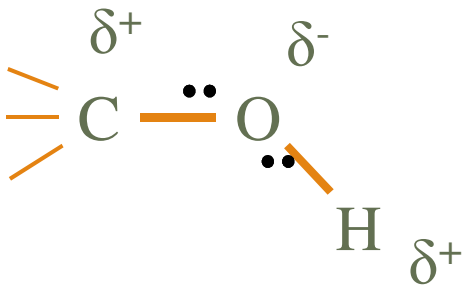
Hydroxyderivatives

Alifatic: **alcohols**

Aromatic: **phenols**

C-OH bond is **very polar**

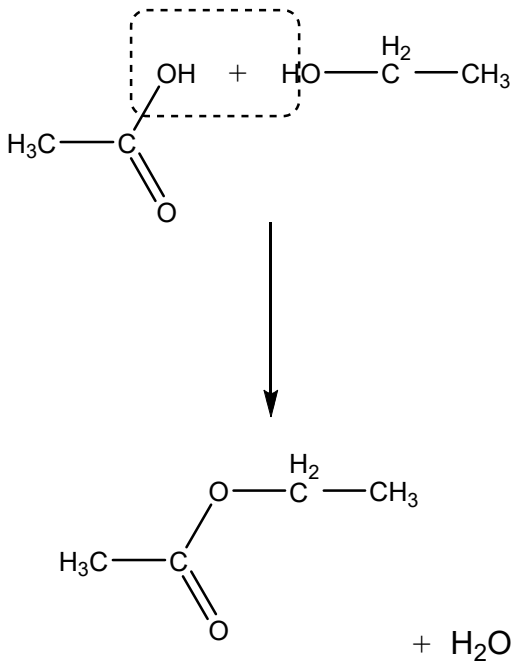
May form hydrogen bonds



Alcohols

- Esterification
- Oxidation
- Alcoholates

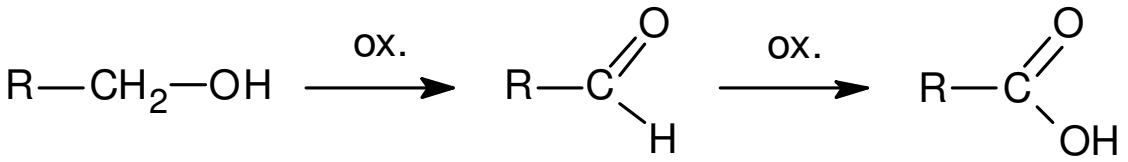
Esterification



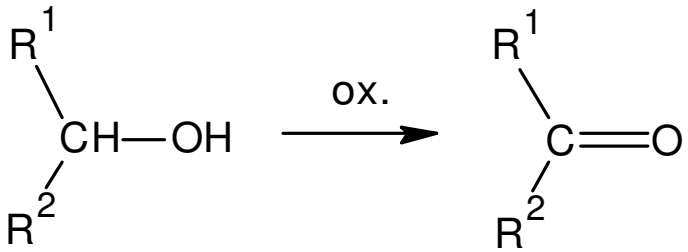
Back reaction:
Hydrolysis of an ester

Oxidation of alcohols

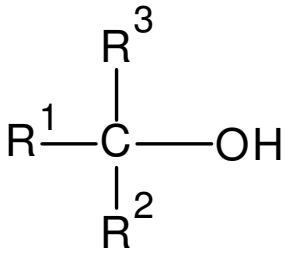
Primary



Secondary

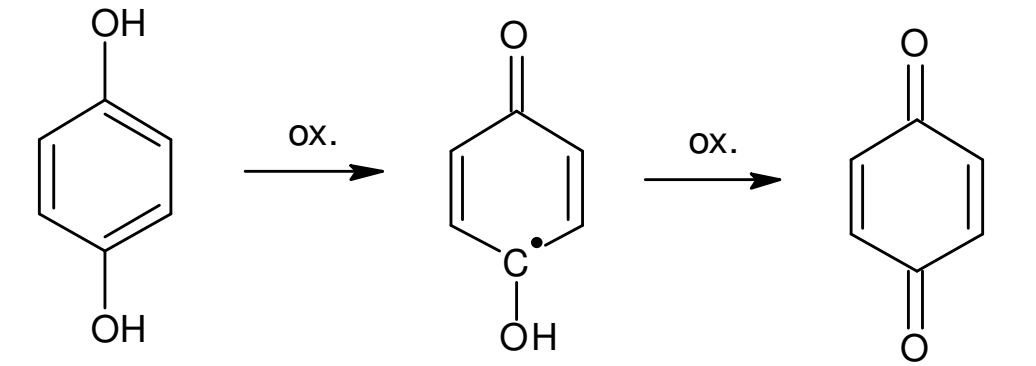


Tertiary



Phenols

- More acidic (phenolates)
- Oxidation to (semi)quinones



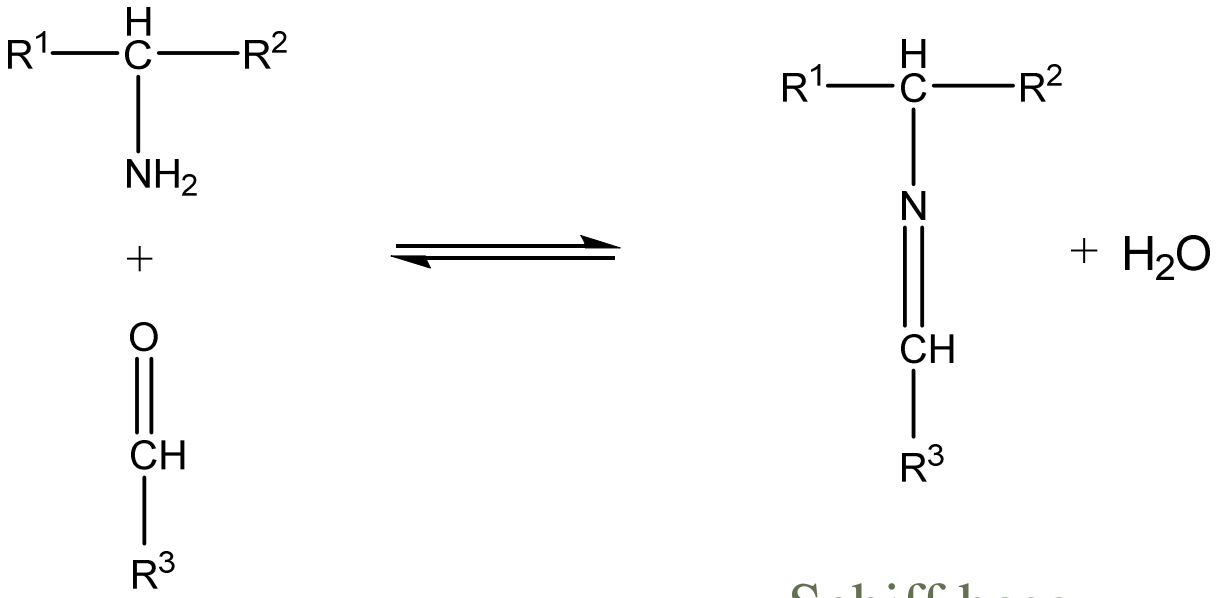
Hydroquinone Phenoxy-radical Benzoquinone

Oxoderivatives

- Aldehydes
- Ketones

- Cannot form hydrogen bridges easily
- Oxidoreductions
- Formation of Schiff base

Schiff base

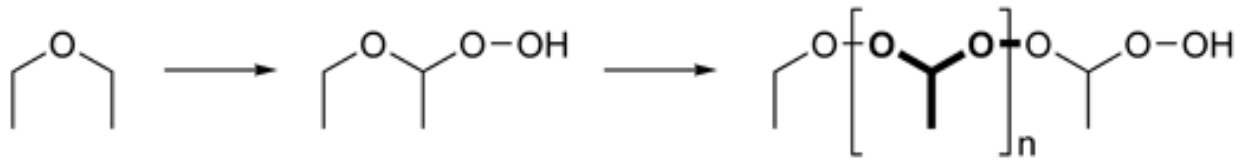


Schiff base
(secondary aldimine)

Ethers

- Group R-O-R
- Less polar

- Simple: explosive



Diethyl ether

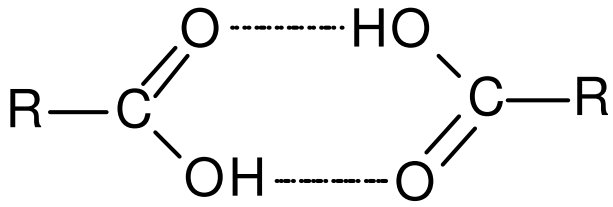
Diethylether hydroperoxide

Diethylether peroxide

Carboxylic acids

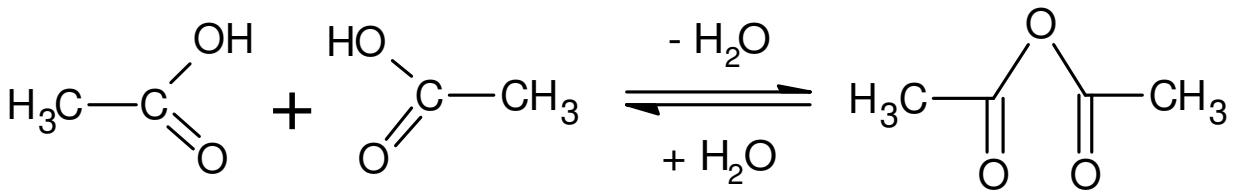
- Weak acids
- Higher fatty acids

- Hydrogen bonds – can form dimers



Carboxylic acids

- Reduction
- Decarboxylation
- Anhydrides



Acetic acid

Acetanhydride