

MACROMOLECULES

lecture for physics and biophysics students

2018. winter semester – 24. September

 **Jenő KÜRTI**

Eötvös Loránd University

Institute of Physics

Department of Biological Physics

Nobel Prize in Chemistry, 2000
for the discovery of **polyacetylene** (1974)
(prototype of the family of **conjugated polymers**)



Alan J. Heeger
1936-

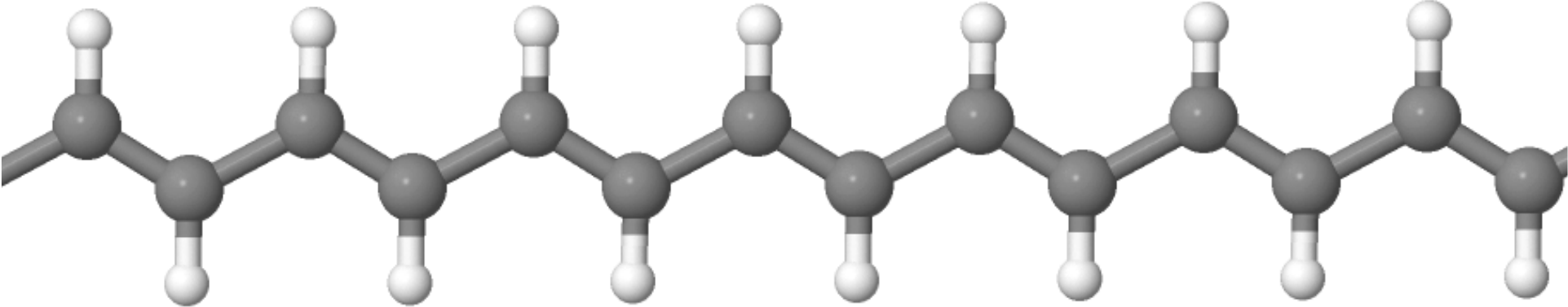


Alan G. MacDiarmid
1927-2007

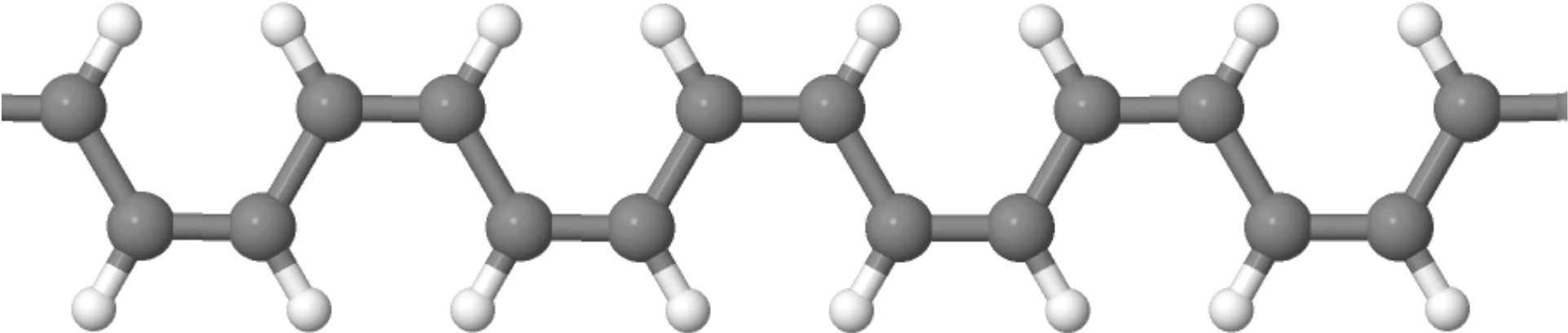


Hideki Shirakawa
1936-

polyacetylene

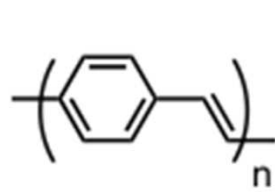
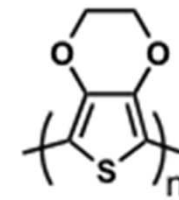
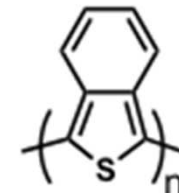
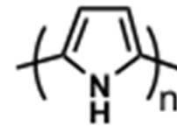
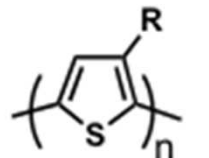
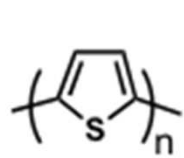
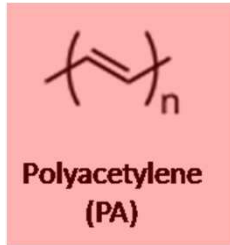


trans (trans-transoid)

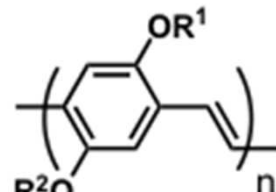


cis (cis-transoid)

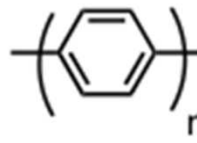
Common conjugated polymers



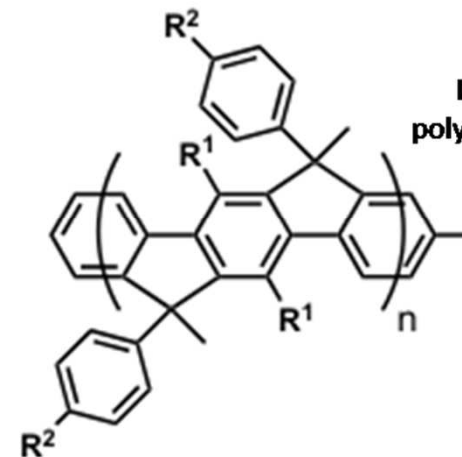
Poly(4-phenyl-1,3-butadiene) (PPV)



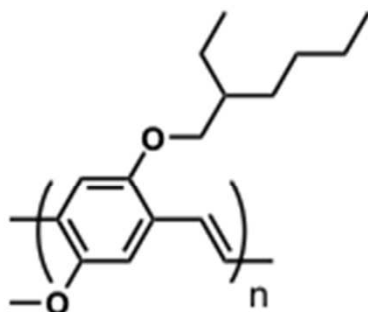
Poly(2,5-dialkoxy-1,3-butadiene) (eg. MEH-PPV)



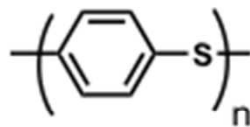
Poly(p-phenylene) (PPP)



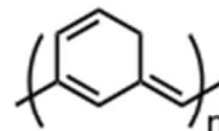
Ladder-type poly(p-phenylene) (LPPP)



Poly(2,5-dialkoxy-1,3-butadiene) (eg. MEH-PPV)

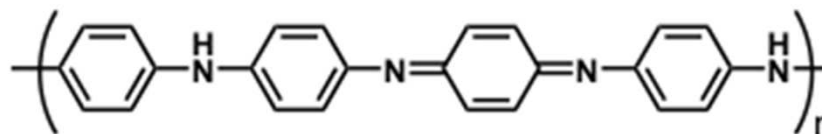
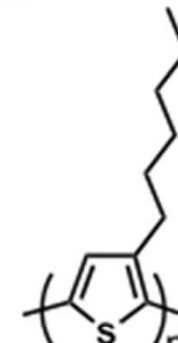


Poly(p-phenylene sulphide) (PPS)



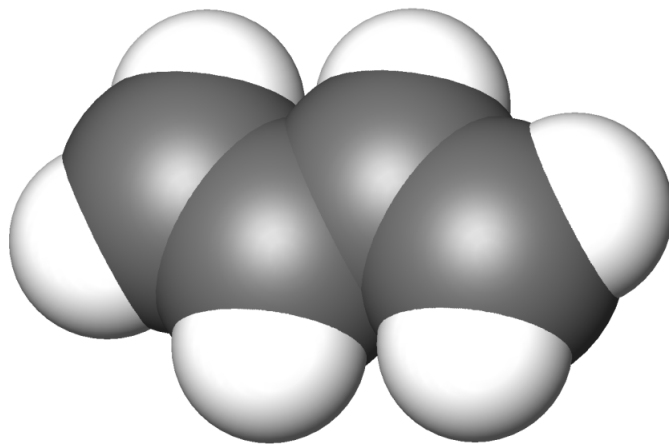
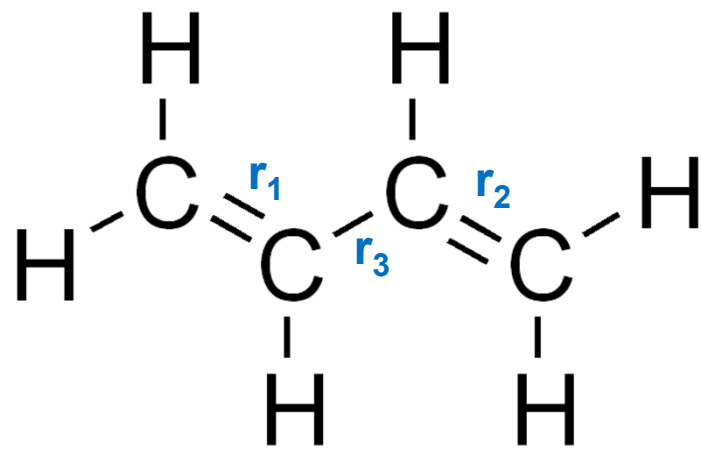
Polyheptadiyne (PHT)

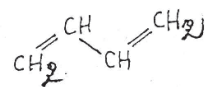
Poly(3-hexylthiophene) (P3HT)



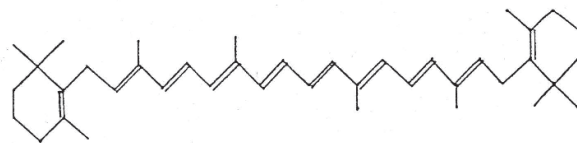
Polyaniline, PANI

trans-butadiene

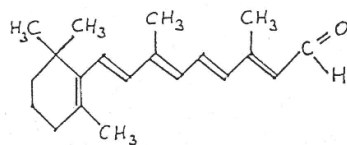




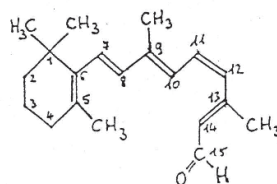
butadién



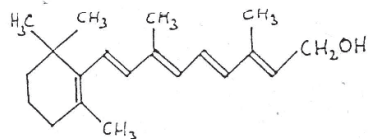
dihidro- β -karotin (8)



all-transz-retinál

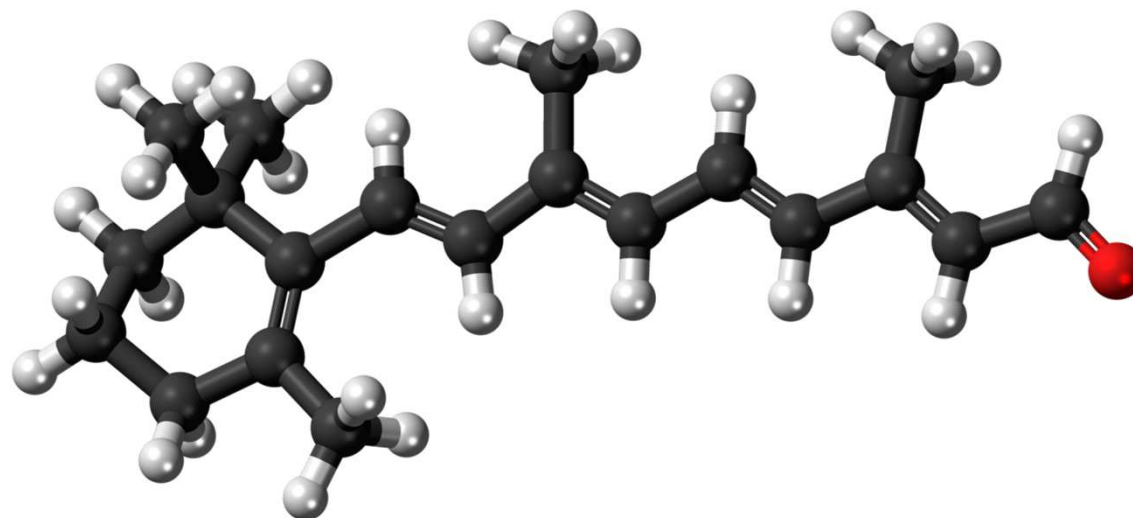


11-cisz-retinál

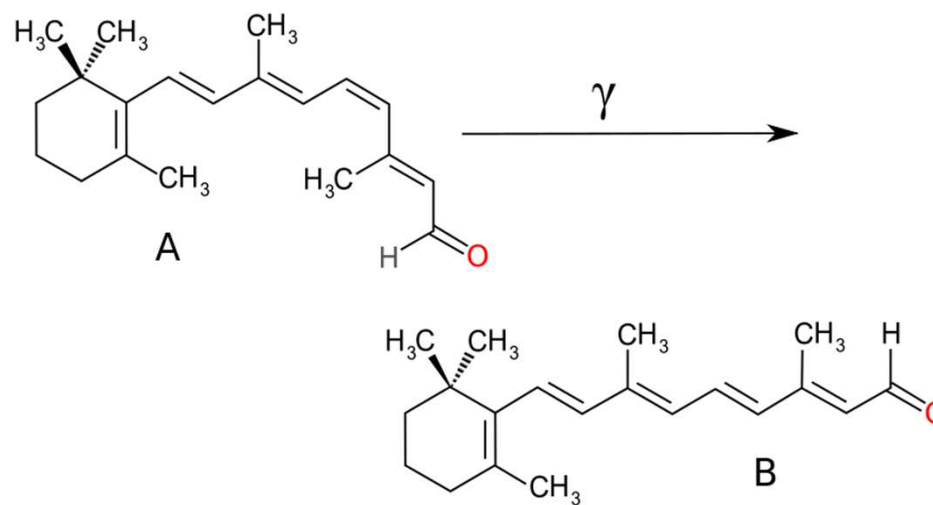


all-transz-retinol (A-vitamin)

Példák: konjugált kismolekulákra

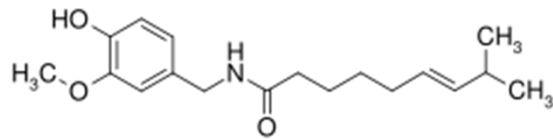


All-trans retinal ($C_{20}H_{28}O$)

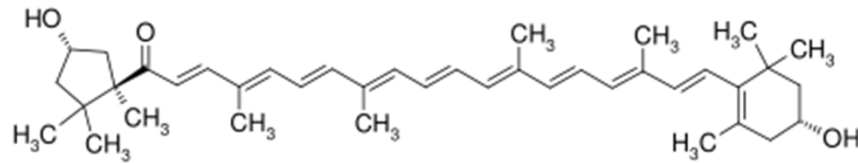


Retinal: cis (A) – trans (B) transition

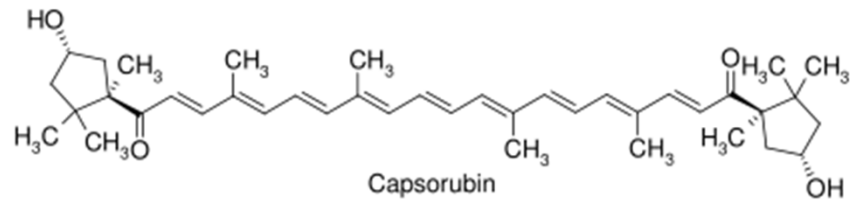
Paprika ...



Capsaicin

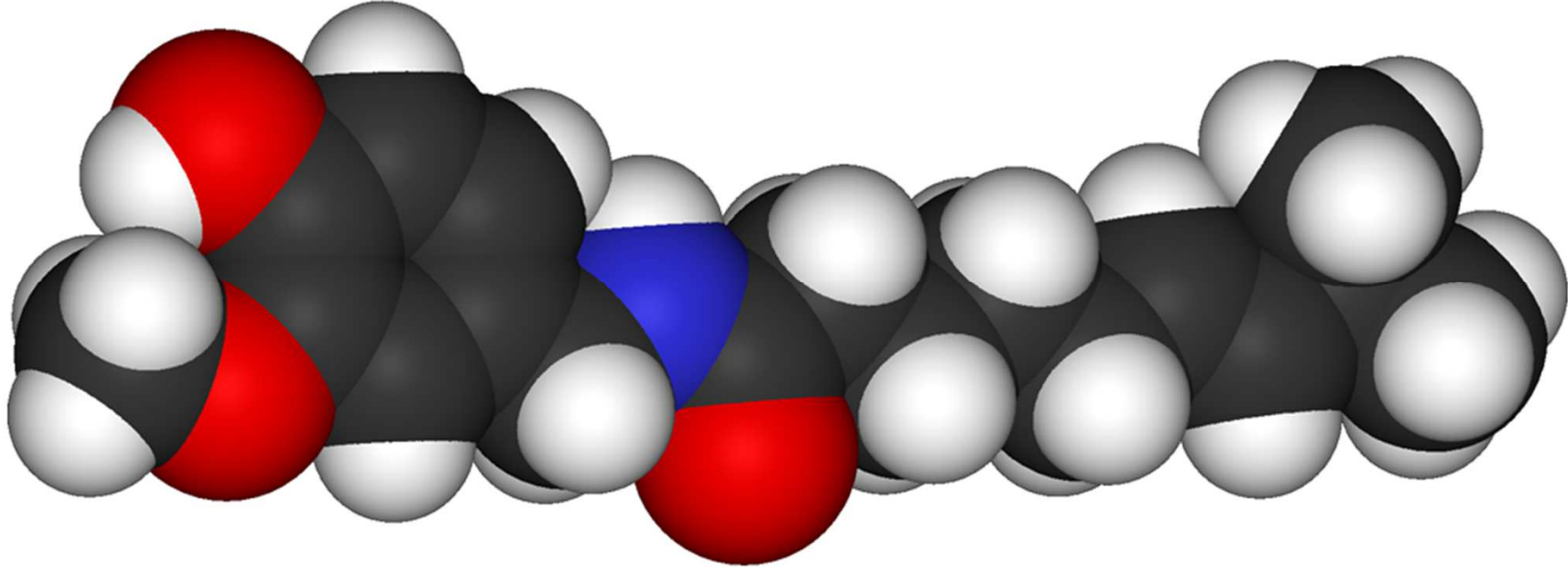


Capsanthin

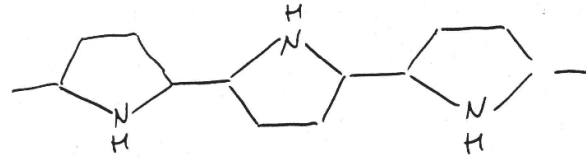


Capsorubin

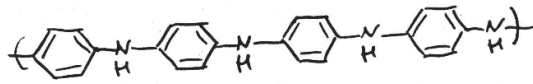
Capsaicin (C₁₈H₂₆O₃N)



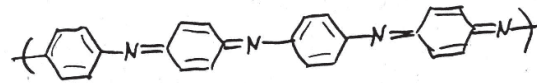
polipirrol



polianilin



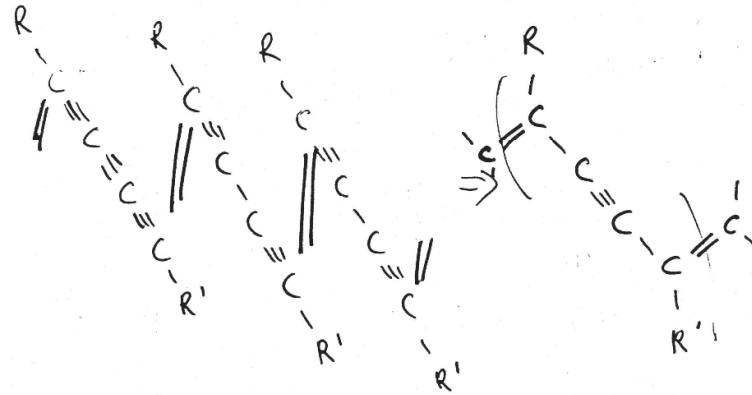
leuco emeraldin



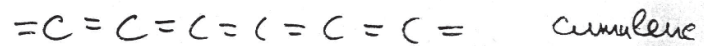
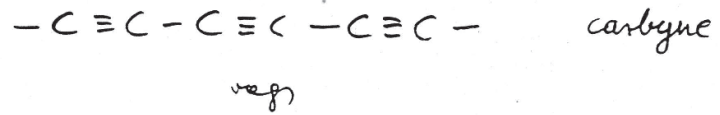
pernigraniline.

három kötéssel tartalmazó polimerek

- polidiacetilén(ek)



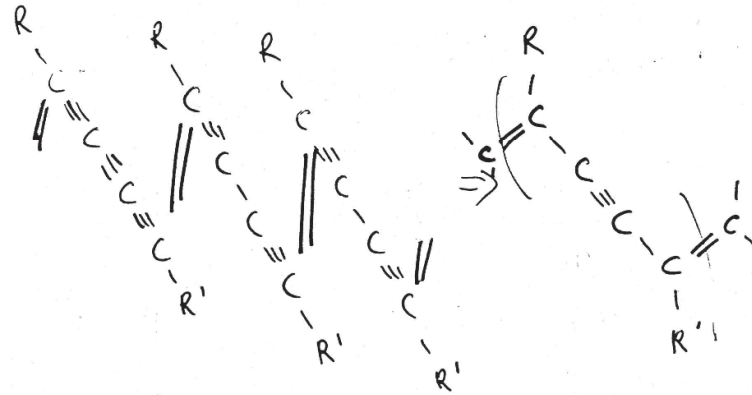
- polycarbyne



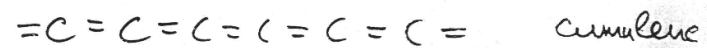
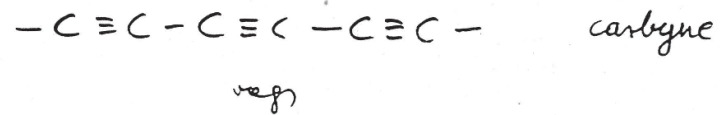
három kötéssel tartalmazó polimerek

- polidiacetilén(ek)

<https://en.wikipedia.org/wiki/Polydiacetylenes>

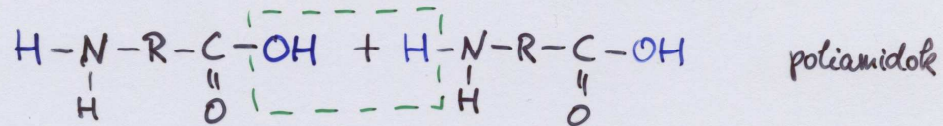
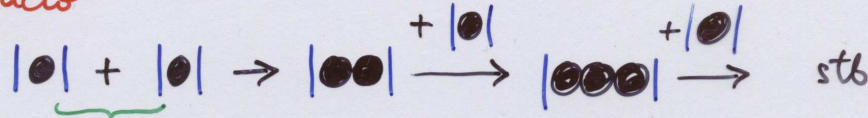


- polycarbyne

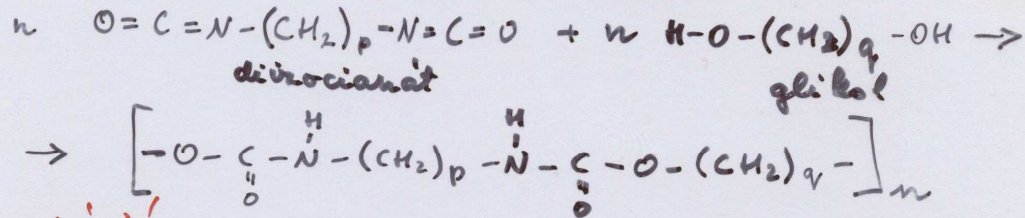


POLIMEREK ELŐÁLLÍTÁSA

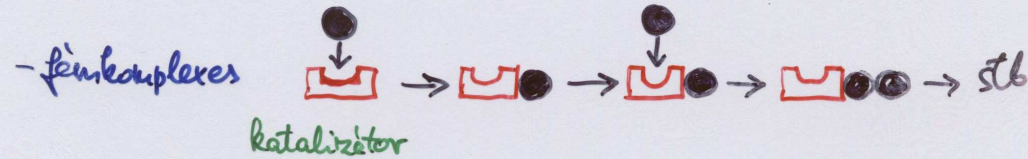
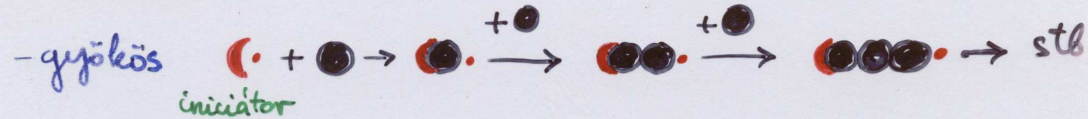
polikondenzáció



poliaddíció

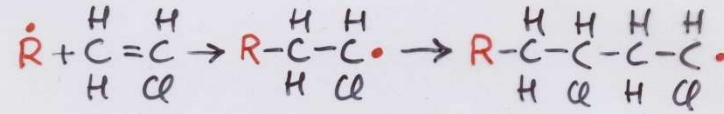


polimerizáció



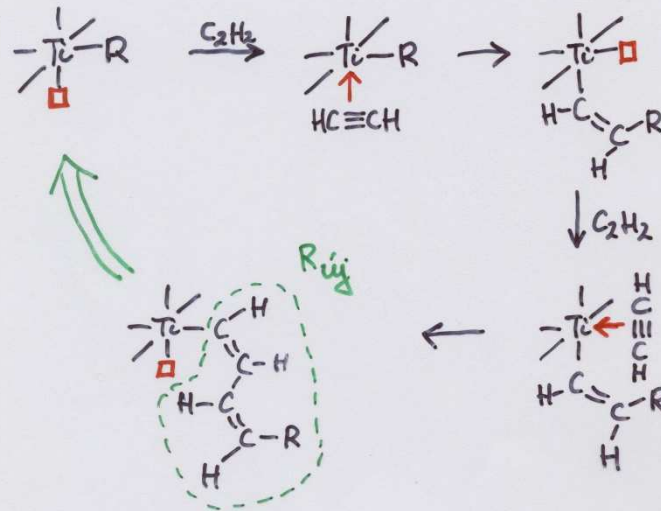
Példák polimerizációra

gyökös



PVC

fémkomplexes

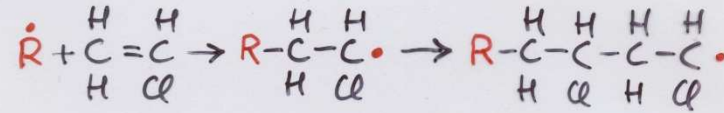


Poliacetilén

(Ziegler-Natta katalizátor: $\text{AlEt}_3 + (\text{Bu})_2\text{TiCl}_2$ toluolban)

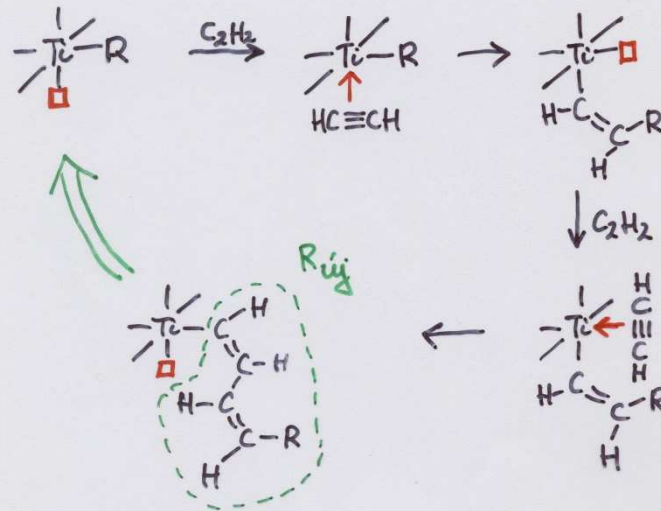
Példák polimerizációra

gyökös



PVC

fémkomplexes



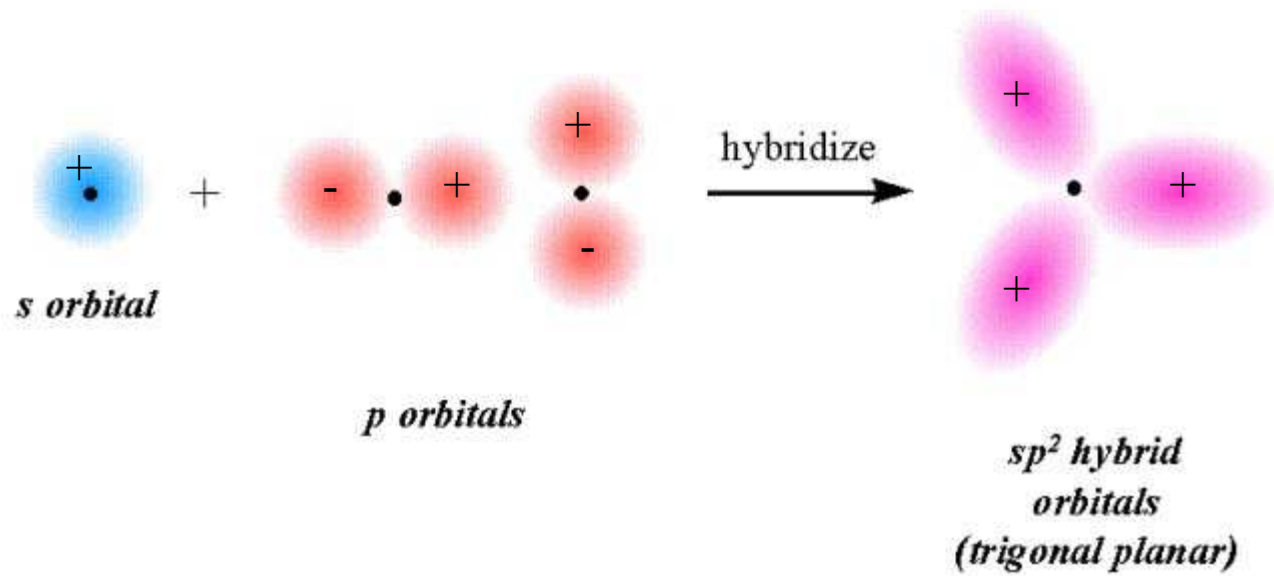
Poliacetilén

[https://en.wikipedia.org/wiki/Ziegler
%E2%80%93Natta_catalyst](https://en.wikipedia.org/wiki/Ziegler%E2%80%93Natta_catalyst)

(Ziegler-Natta katalizátor: $\text{AlEt}_3 + (\text{Bu})_2\text{TiCl}_2$ toluolban)

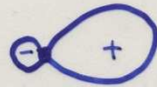
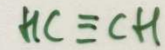
KITÉRŐ

(hibridizáció)

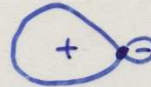


s-p hibridpályák

sp (lineáris)



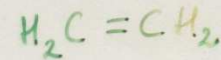
$$\frac{1}{\sqrt{2}}(s + p_z)$$



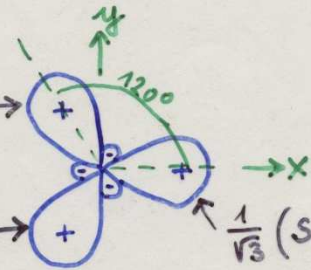
$$\frac{1}{\sqrt{2}}(s - p_x)$$

→ z

sp² (trigonális)



$$\frac{1}{\sqrt{3}}(s - \frac{1}{\sqrt{2}}p_x + \frac{\sqrt{3}}{2}p_y) \rightarrow$$



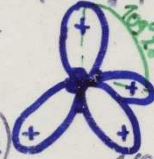
$$\frac{1}{\sqrt{3}}(s - \frac{1}{\sqrt{2}}p_x - \frac{\sqrt{3}}{2}p_y) \rightarrow$$

$$\frac{1}{\sqrt{3}}(s + \sqrt{2} \cdot p_x)$$

sp³ (tetragonális)



$$\frac{1}{2}(s + p_x + p_y + p_z)$$

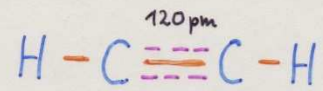


$$\frac{1}{2}(s - p_x - p_y + p_z)$$

$$\frac{1}{2}(s + p_x - p_y - p_z)$$

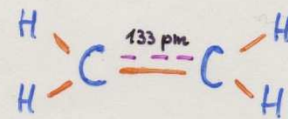
$$\frac{1}{2}(s - p_x + p_y - p_z)$$

sp^1 (lineáris) :



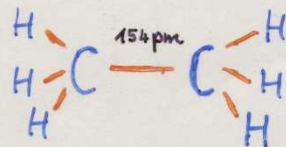
acetilén

sp^2 (trigonális) :



etilén

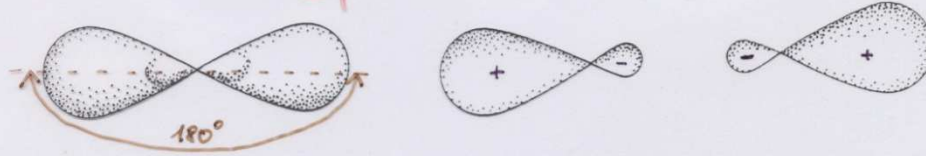
sp^3 (tetragonális) :



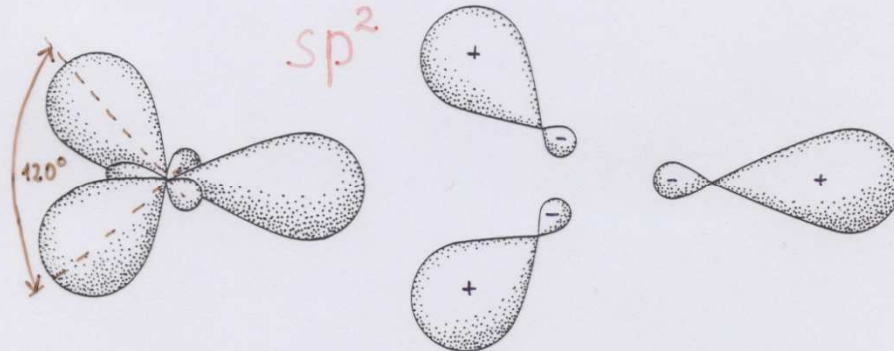
etán

sp - hibridpályák

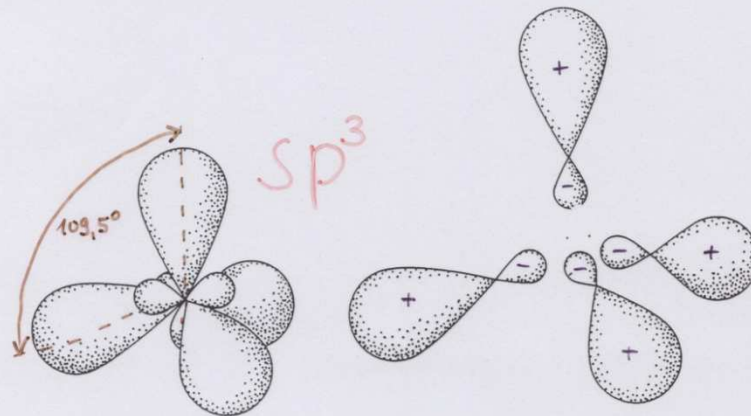
sp¹



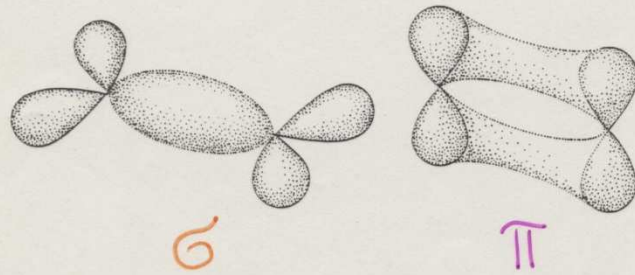
sp²



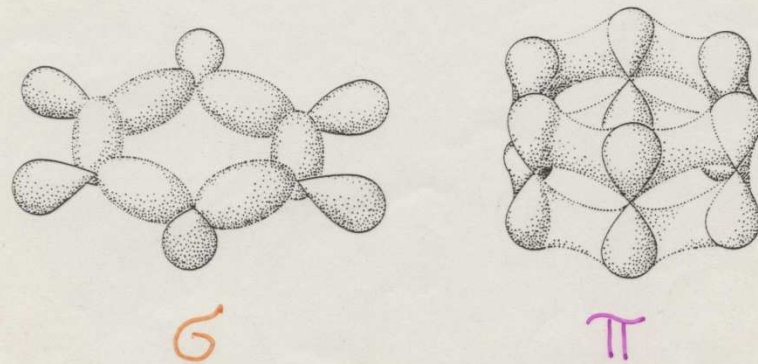
sp³



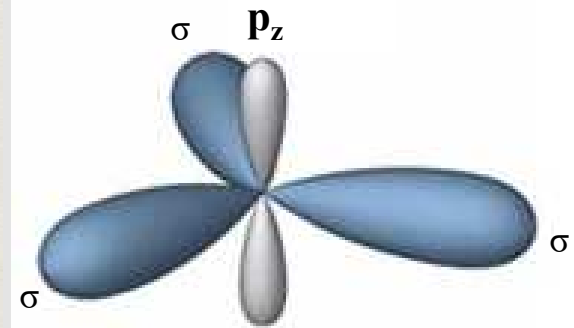
etilén (H₂C=CH₂)



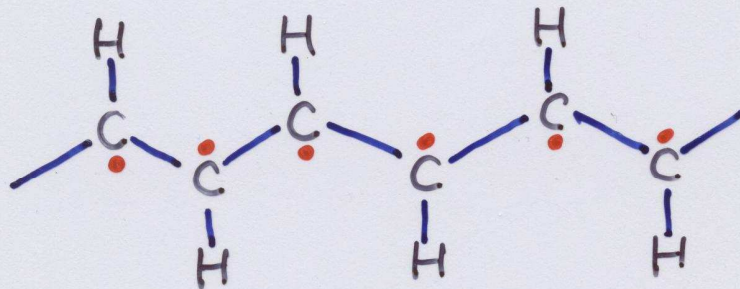
sp^2



benzol (C₆H₆)



trans - POLYACETYLENE



sp^2 hybrid orbital : 3 / carbon atom

→ σ -band, fully occupied

p_z orbital : 1 / carbon atom

→ π -band, half filled