

KONJUGÁLT SZÉNLANCÚ POLIMEREK

Motiváció:

2000 kémiai Nobel-díjasai



Alan J. Heeger

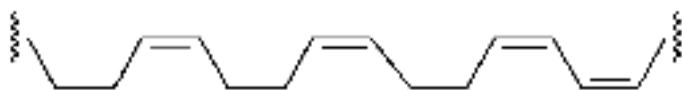


Alan G. MacDiarmid

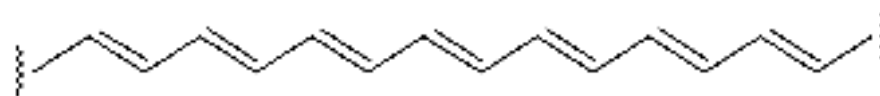


Hideki Shirakawa

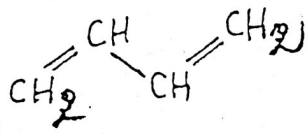
A díjat a vezető polimerek (poliacetilén) felfedezéséért (1974) és kidolgozásáért ítélték oda.



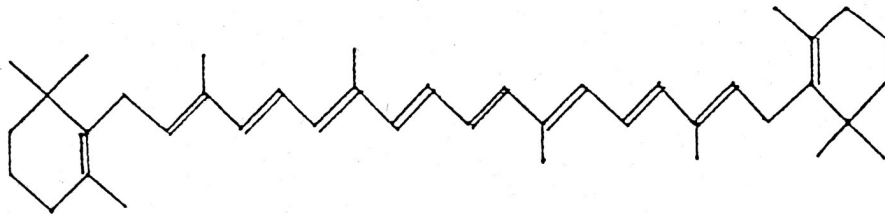
cis z-poliacetilén



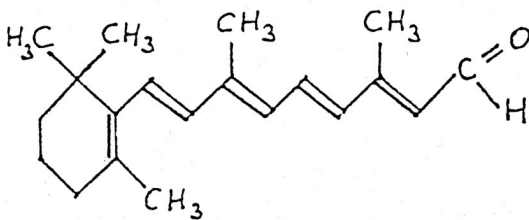
trans z-poliacetilén



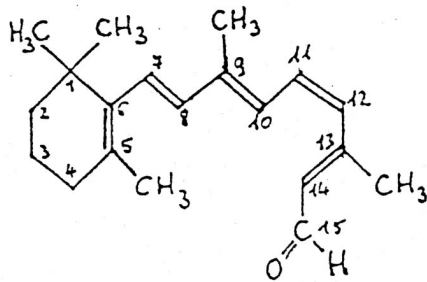
butadién



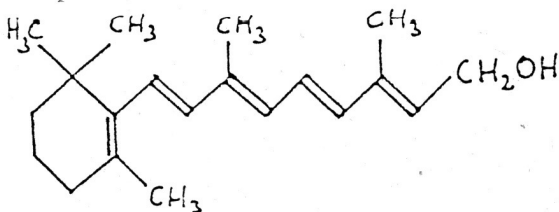
dihidro- β -karotin (8)



all-transz-retinál



11-cisz-retinál

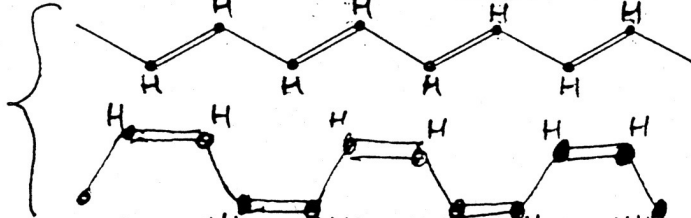


all-transz-retinol (A-vitamin)

Példák konjugált kismolekulákra

KONJUGÁLT SZÉNLANCÚ POLIMEREK

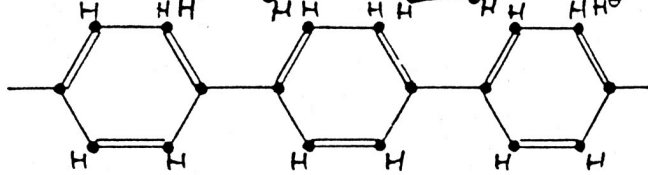
$(CH)_x$



trans-polyacetylene

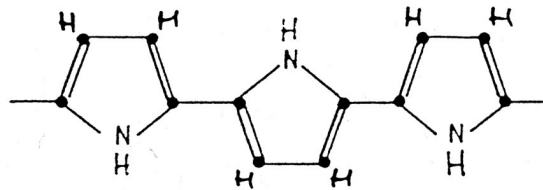
cis-polyacetylene

PPP



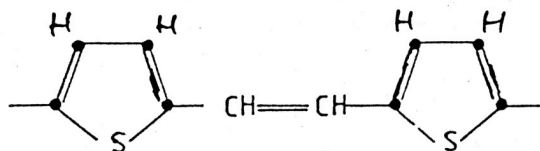
polyparaphenylene

PPY



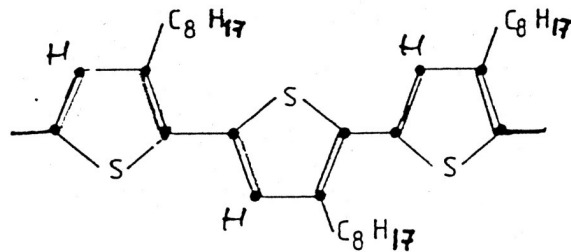
polypyrrole

PTV



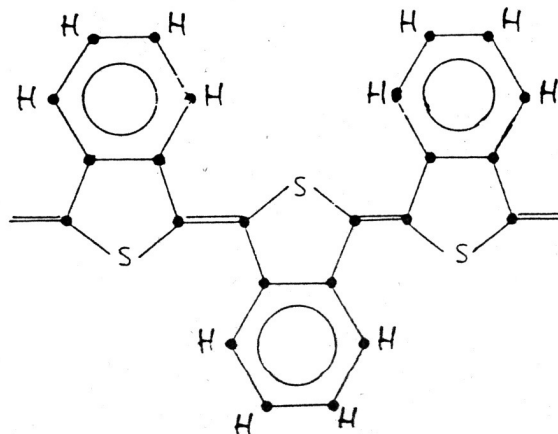
poly(2,5-thienylene vinylene)

POT



polyoctylthiophene

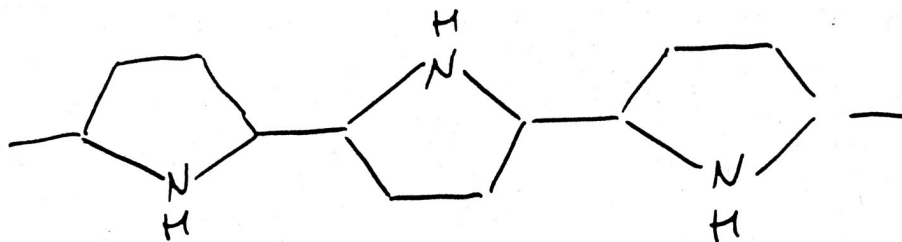
PITN



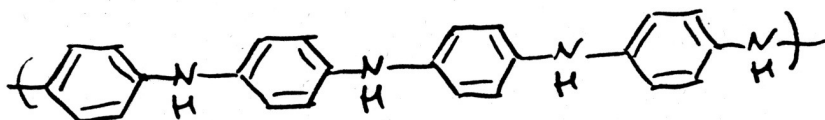
polyisothianaphthene

poly(1,3-benzothienophene)

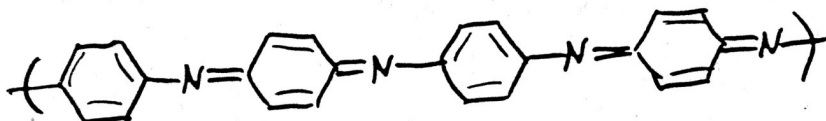
polipirrol



polianilin



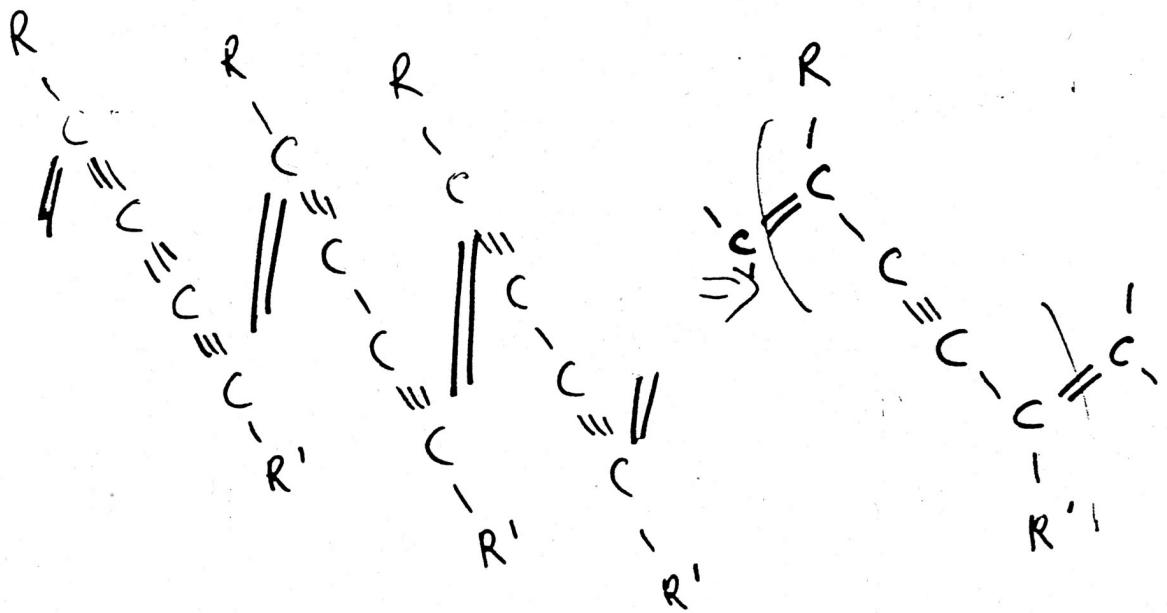
leuco emeraldin



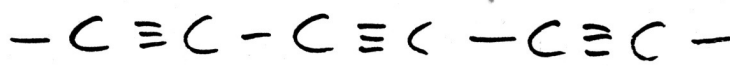
pernigraniline.

Három kötet tartalmazó polimerek

- polidiacetilén(ek)

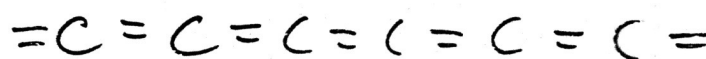


- polycarbyne



carbyne

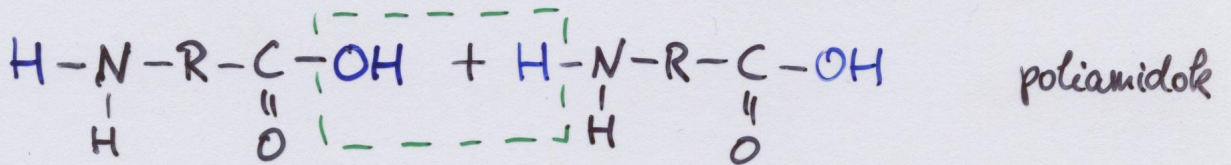
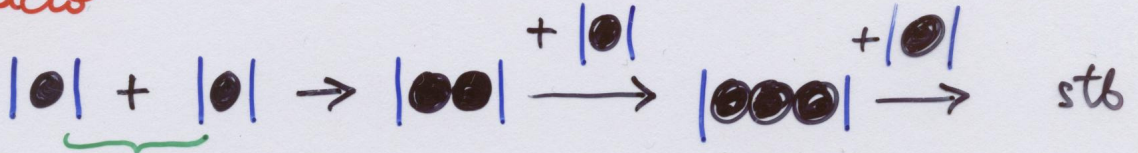
veg



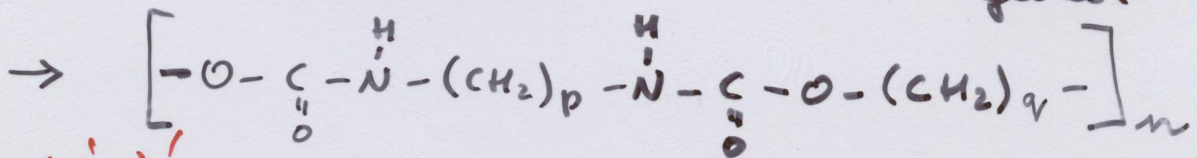
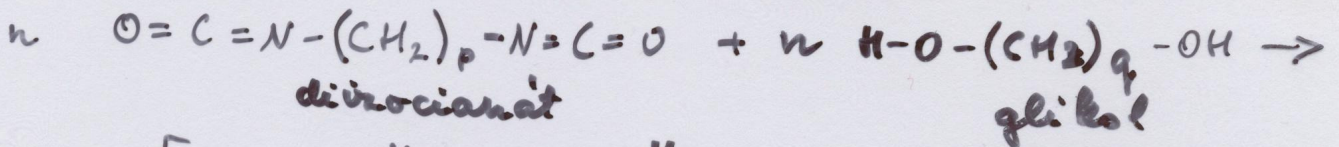
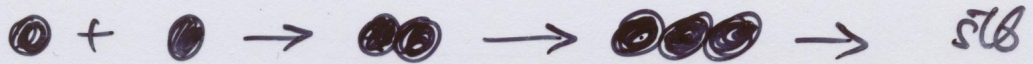
cumulene

POLIMEREK ELŐÁLLÍTÁSA

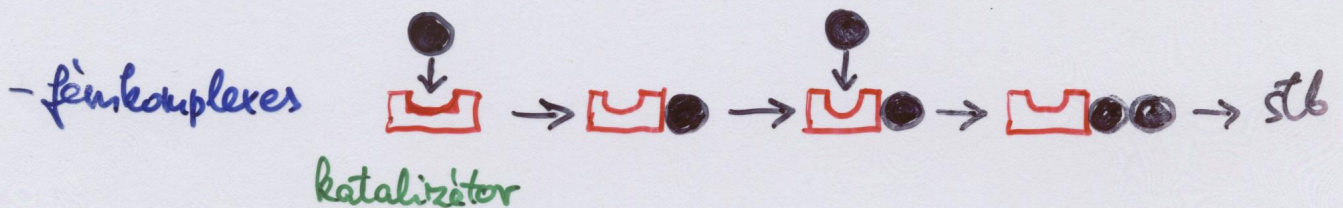
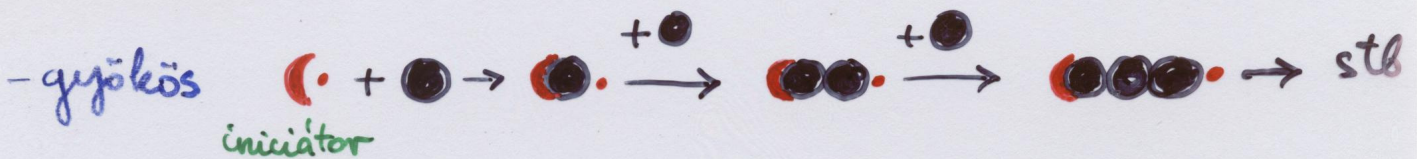
polikondenzáció



poliaddíció

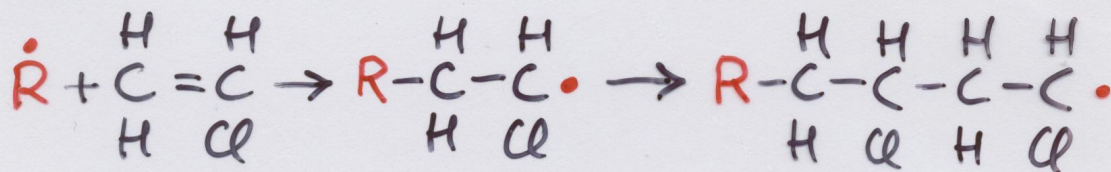


polimerizáció



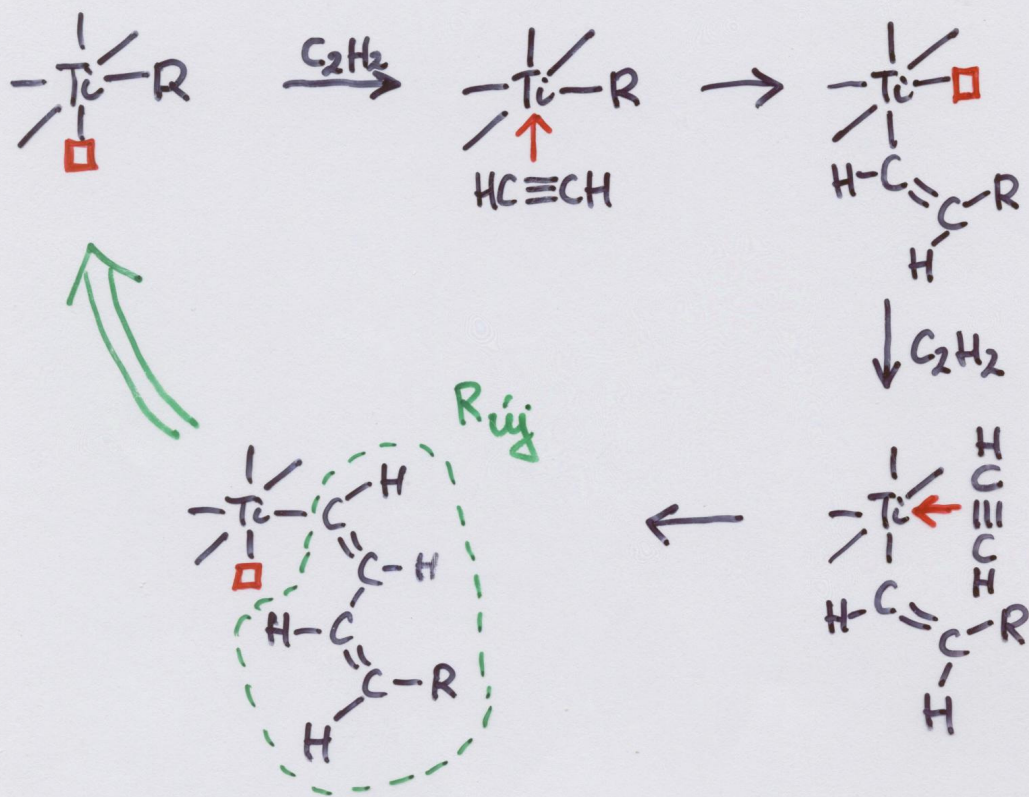
Példák polimerizációra

gyökös



PVC

fémkomplexes

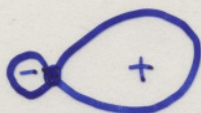
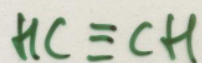


Poliacetilén

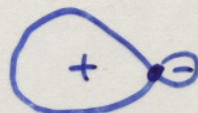
(Ziegler-Natta katalizátor: $\text{AlEt}_3 + (\text{Bu})_2\text{TiO}_2$ toluolban)

s-p hibridpályák

sp (lineáris)



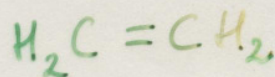
$$\frac{1}{\sqrt{2}}(s + p_z)$$



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

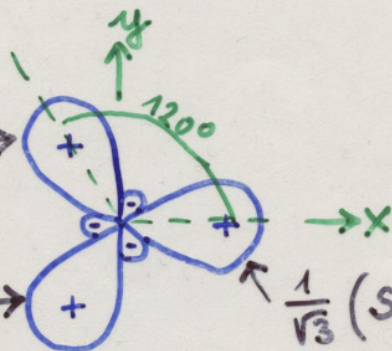
→ z

sp² (trigonális)



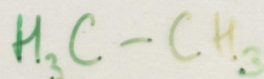
$$\frac{1}{\sqrt{3}}\left(s - \frac{1}{2}p_x + \sqrt{\frac{3}{2}}p_y\right)$$

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



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

sp³ (tetragonális)

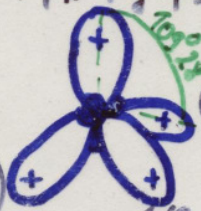


$$\frac{1}{2}(s + p_x + p_y + p_z)$$

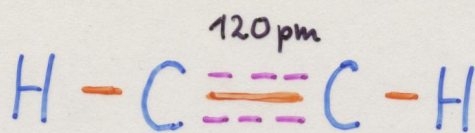
$$\frac{1}{2}(s - p_x + p_y - p_z)$$

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

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

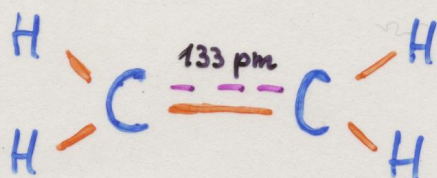


sp^1 (lineáris) :



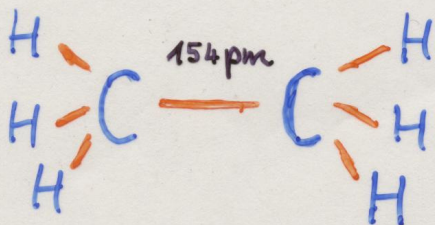
acetilén

sp^2 (trigonális) :



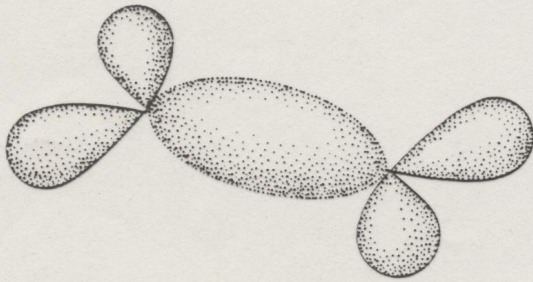
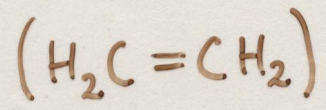
etilén

sp^3 (tetragonális) :

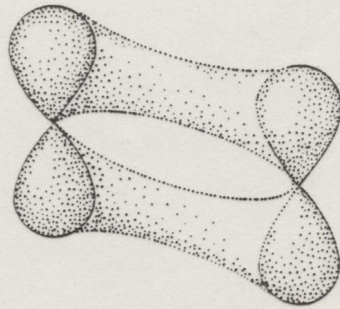


etán

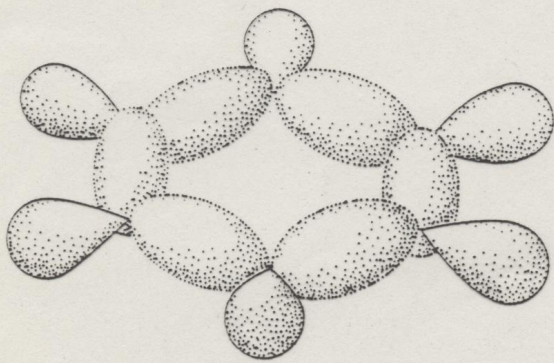
etilén



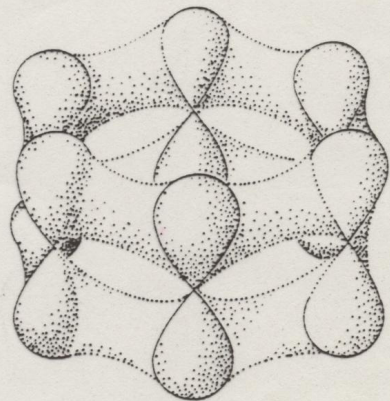
σ



π

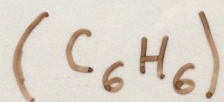


σ



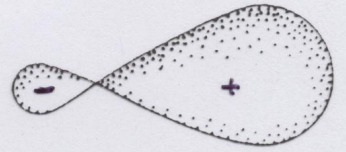
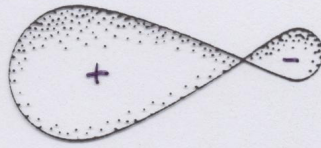
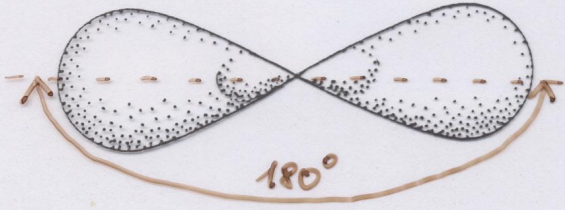
π

benzol

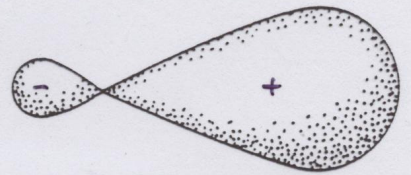
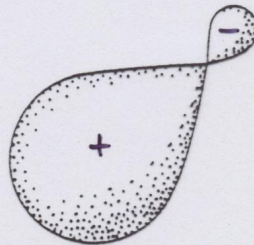
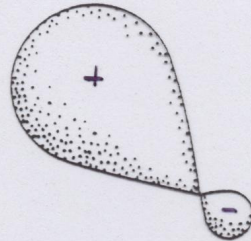
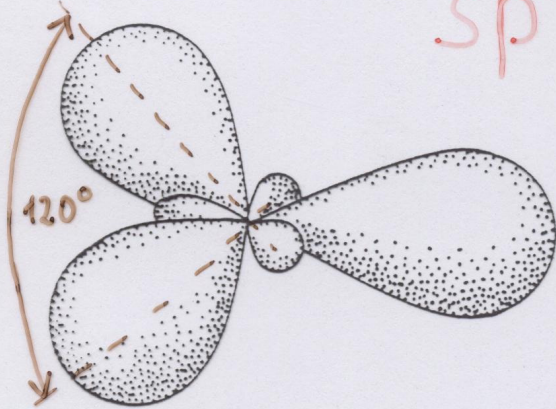


sp - hibridpályák

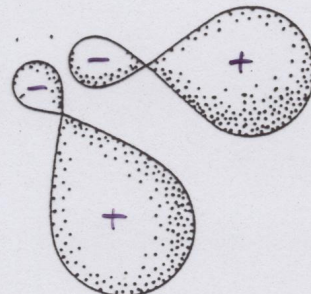
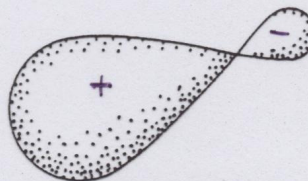
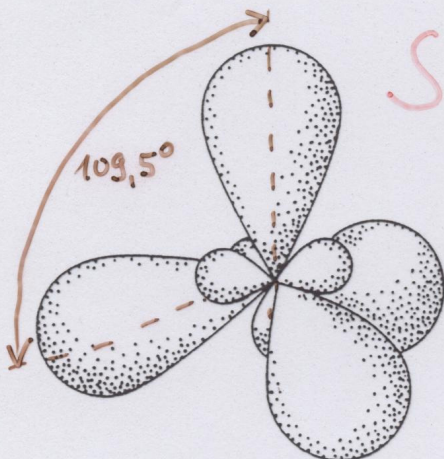
sp¹



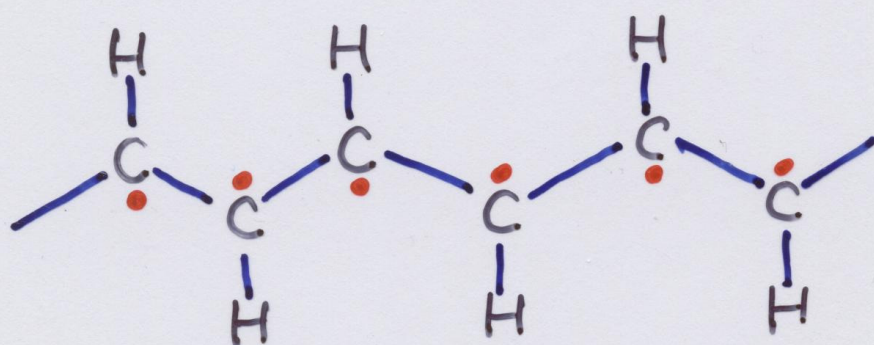
sp²



sp³



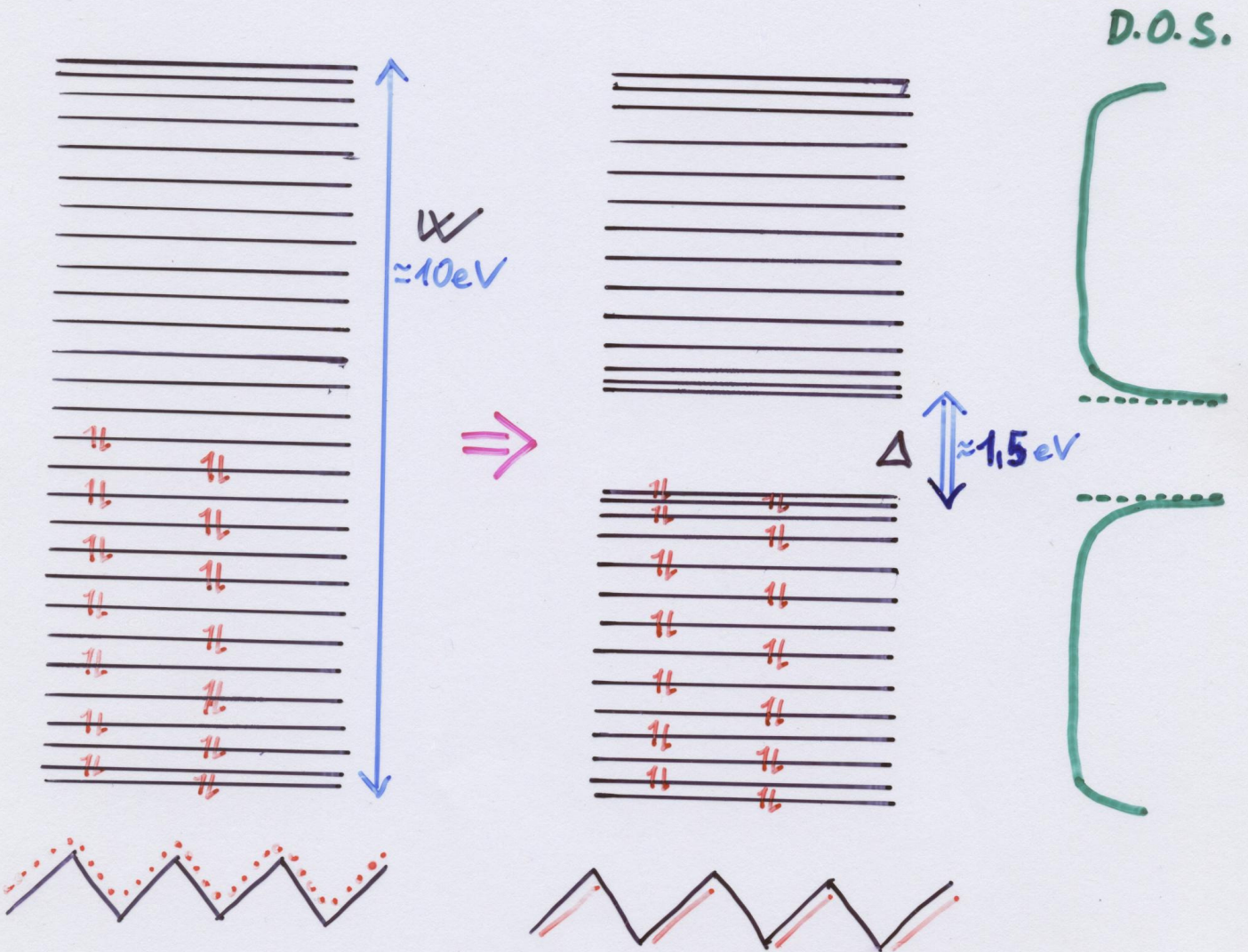
trans - POLYACETYLENE



sp^2 hybrid orbital : 3 / carbon atom
→ σ -band, fully occupied

p_z orbital : 1 / carbon atom
→ π -band, half filled

trans - PA



$$\pi_{||} \approx 1,36 \text{ \AA}$$

$$\pi_{\perp} \approx 1,44 \text{ \AA}$$