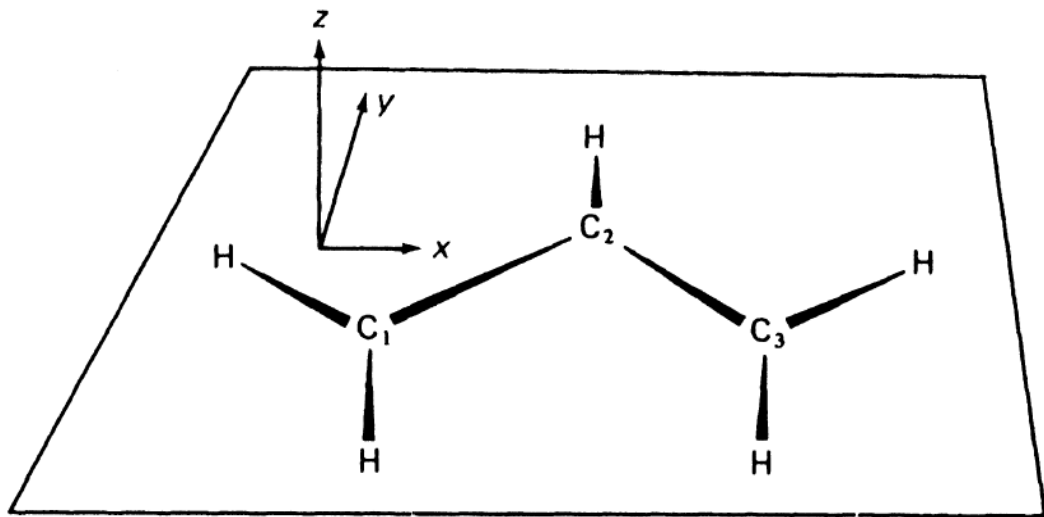


C9930, 3. přednáška, 17. 3. 2021

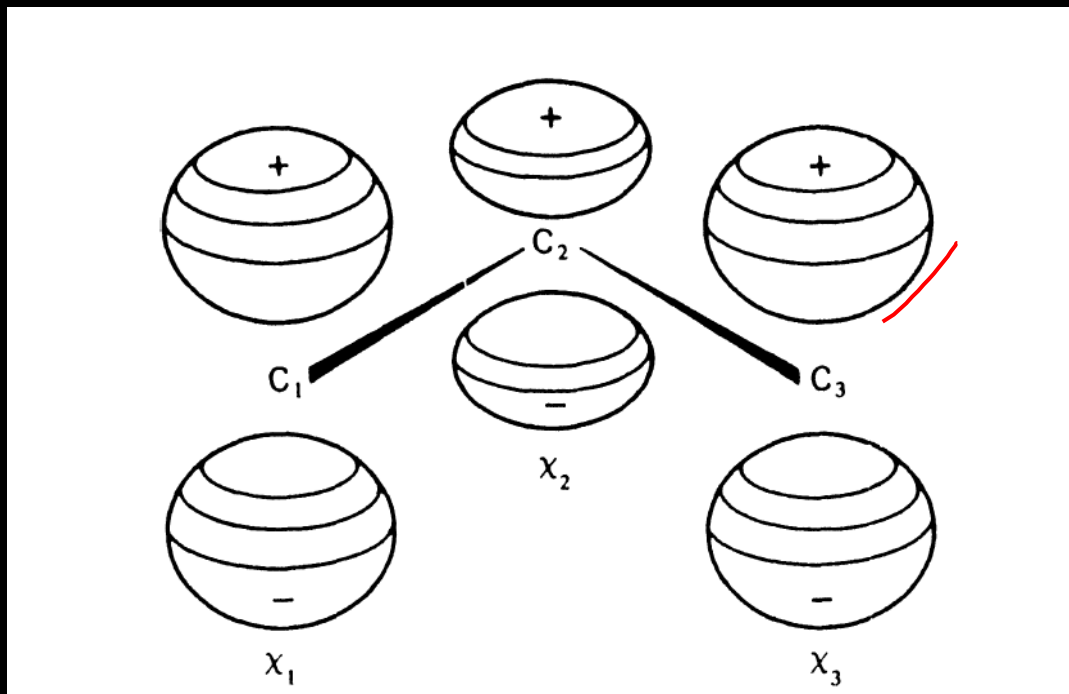
Obyčejná Hückelova metoda:  
*Předpoklady a vztah k experimentu*  
(Lowe 8.11-8.13)



Rozšířená Hückelova metoda:  
*Princip*  
(Lowe 10.1)



### 3.1 HMO: Přehled předpokladů a závěrů (Lowe 8-11)



## 3.2 Vztah mezi vazebným řádem a vazebnou délkou (Lowe 8-12)

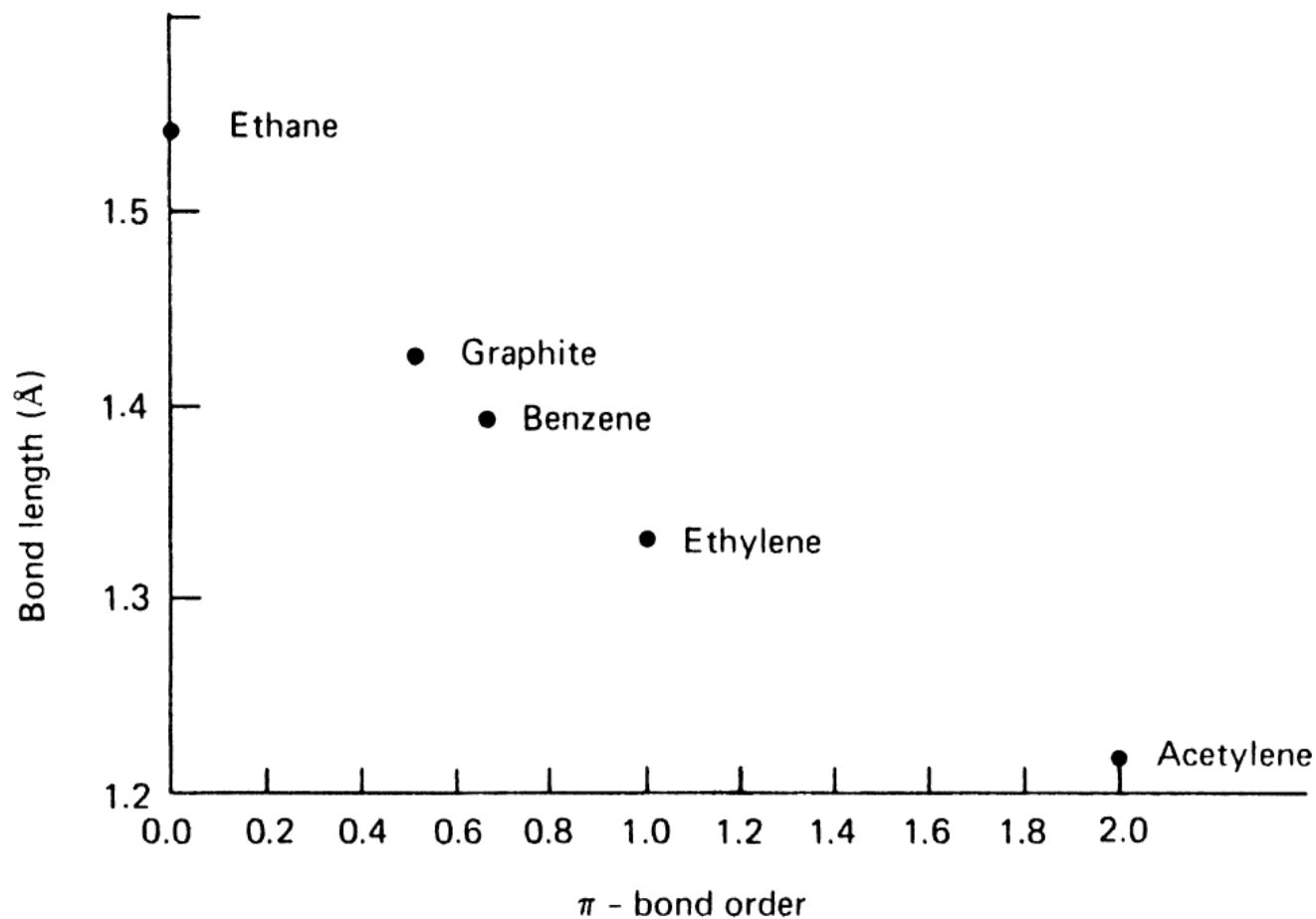
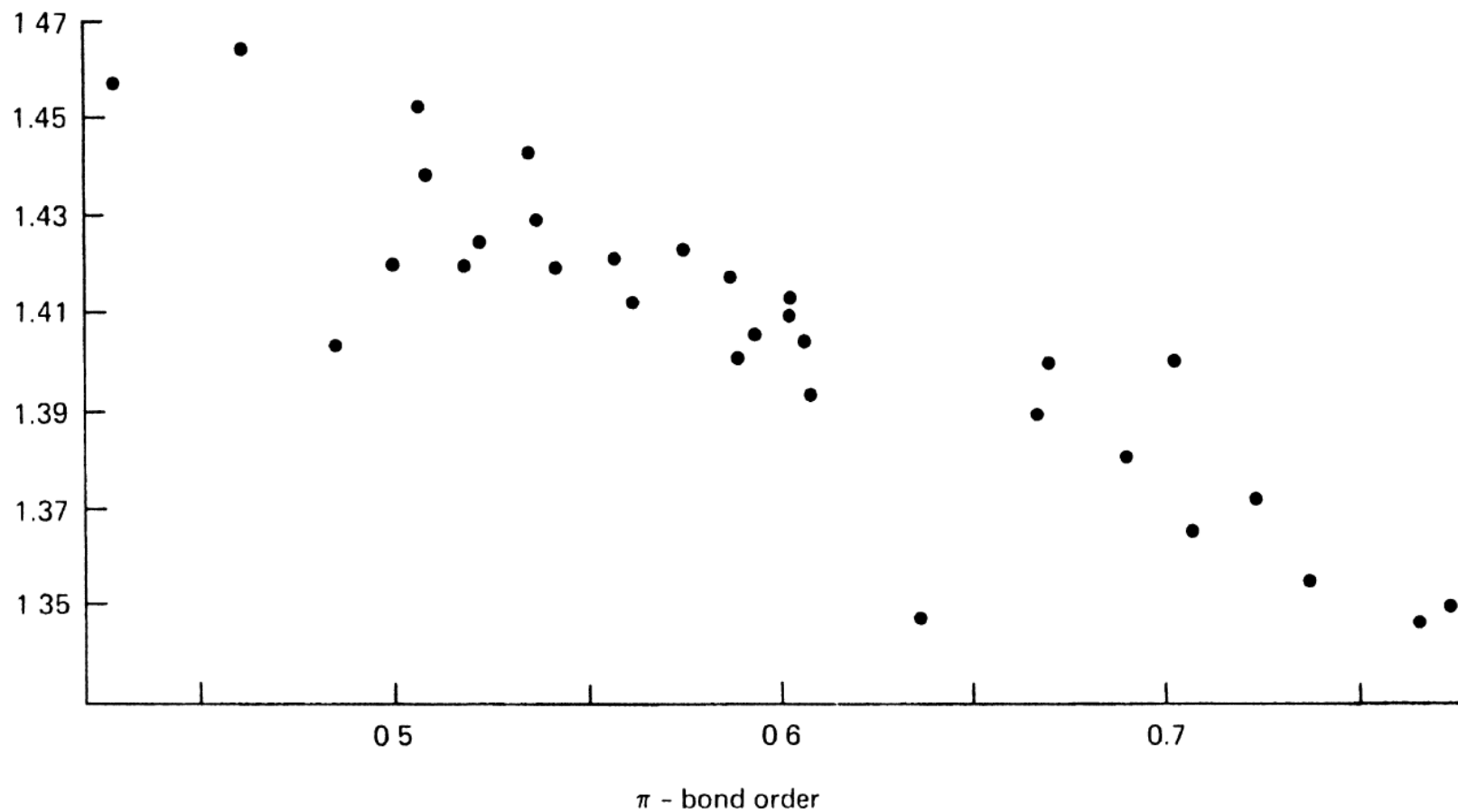
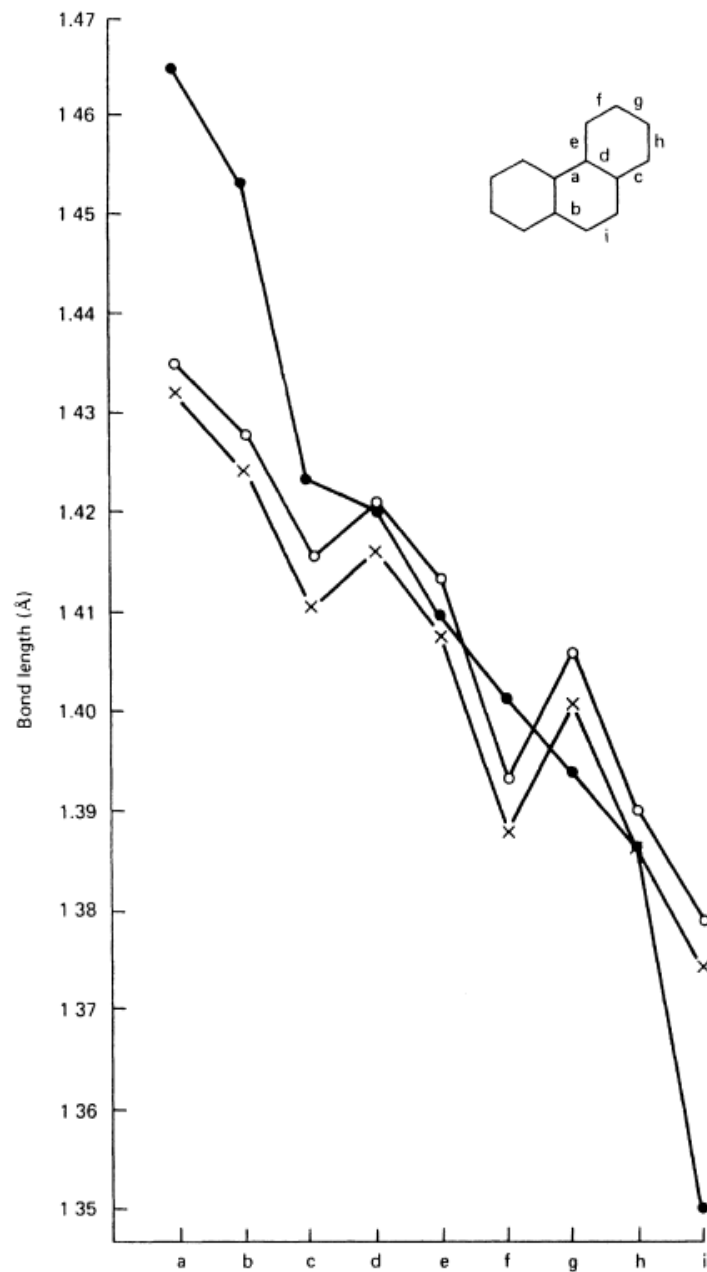


Figure 8-14 ►  $\pi$ -Bond order versus bond length for some simple unsaturated hydrocarbons.

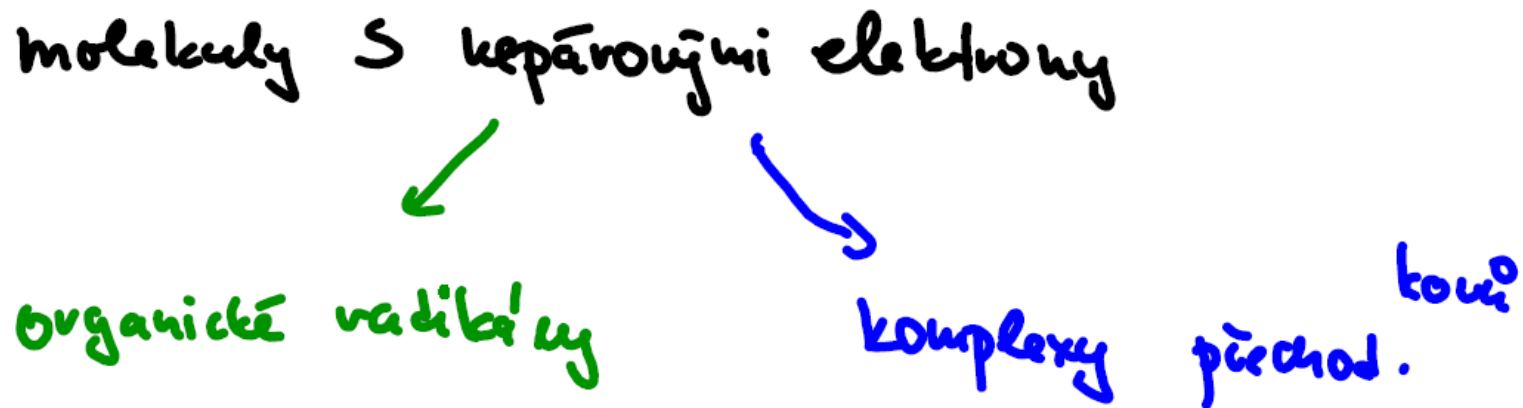


**Figure 8-15** ► Bond lengths versus  $\pi$ -bond orders for benzene, graphite, naphthalene, anthracene, phenanthrene, triphenylene, and pyrene.



**Figure 8-16** ► Theoretical versus experimental bond lengths for phenanthrene in order of decreasing observed length: (●) experimental; (×) theoretical with  $s = 1.54 \text{ \AA}$ ,  $k = 0.765$ ; (○) theoretical with  $s = 1.515 \text{ \AA}$ ,  $k = 1.05$ .

### 3.3 $\pi$ -elektronové hustoty a EPR hyperjemné štěpící konstanty (Lowe 8-13)



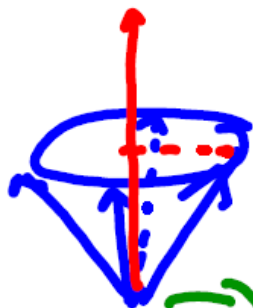
"Nepāroju spin"

$\uparrow$   
 $\alpha$

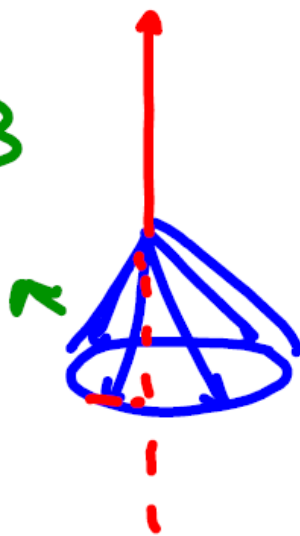
kešo

$\downarrow$   
 $\beta$

$S_z$   
 $\downarrow$   
 $m_s = +\frac{1}{2}$



Bez  
vājšāho  $B$   
skājē  
enerģijē  $S_z$



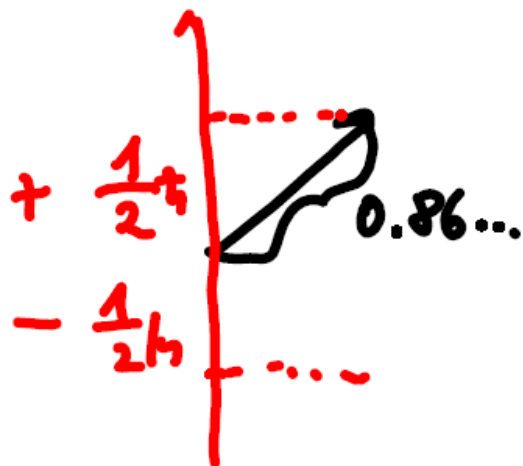
$m_s = -\frac{1}{2}$

$S = \frac{1}{2}$

velikost el. spina:  $\sqrt{S \cdot (S+1)} \hbar$

vel. el. spica  $\sqrt{\frac{1}{2} \left( \frac{1}{2} + 1 \right)} t_1 =$

$$= \sqrt{\frac{1}{2} \cdot \frac{3}{2}} t_1 = \sqrt{\frac{3}{4}} t_1 = \frac{\sqrt{3}}{2} t_1$$



2 možné projekce

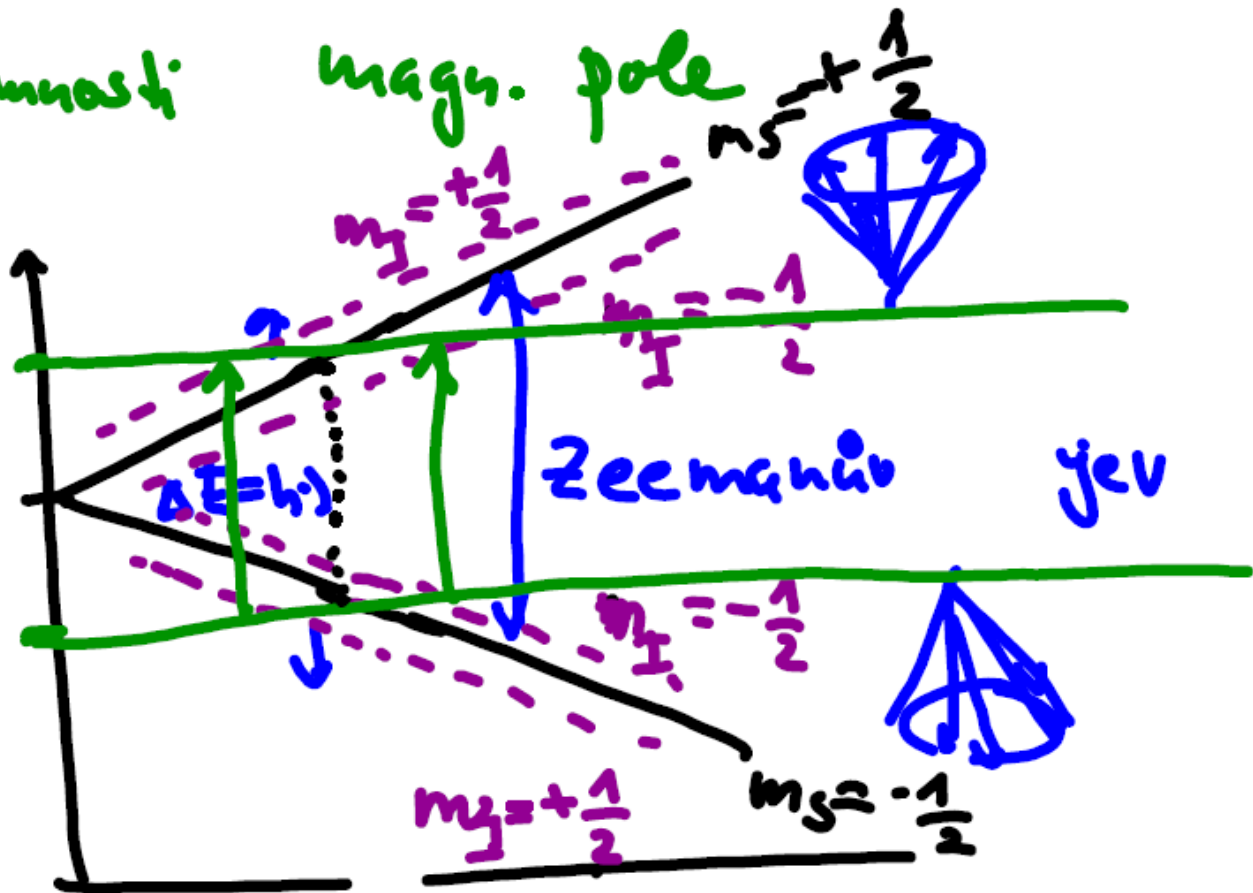
el. spica vypryuvani

$$\approx s = \frac{1}{2} .$$



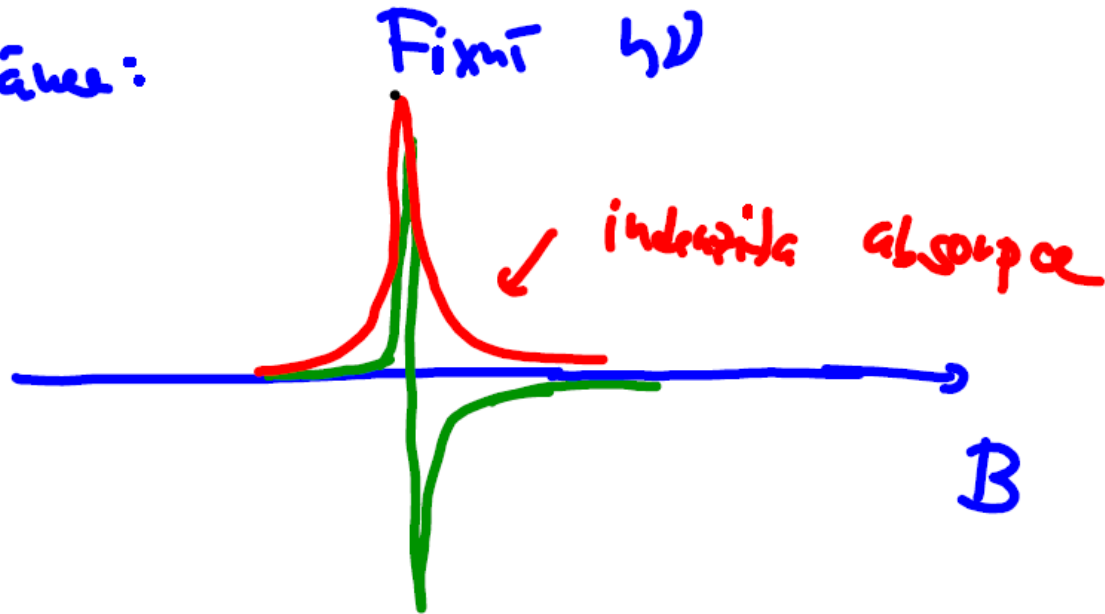
V pīrtomnasti magy. pole  $m_s = +\frac{1}{2}$

enerģie  
elektroni



B

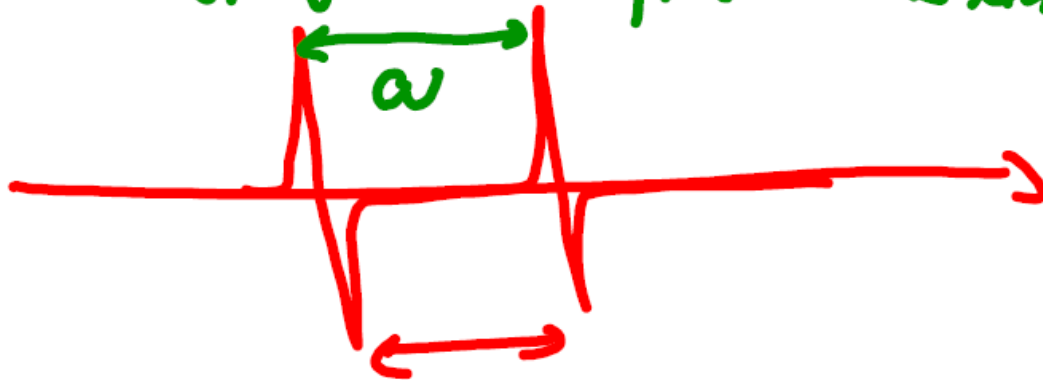
Ošebāvāne:



1. derivāce absorpcijas intensitāte

Skalečnost: izotropne H.

hyperjerna! štipica konstanta



510 Gauss

vezajisi na magnetike indenti.

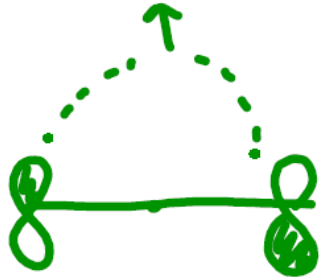
Organické radikály : Je-li nepřiročný elektron

lokalizován v orbitale ar typu  $\pi_1$

hovoříme o tzv.  $\pi$ -radikálech.

Důležitou skupinou jsou planární  $\pi$ -radikály.

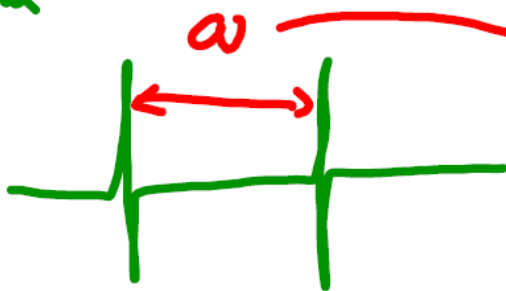
↓  
metoda HMO



## EPR

El. spin. rezonance (el. paramagn. rezonance)

H atom



odpovídá interakci  
mezi spinem elektronu  
a spinem jádra