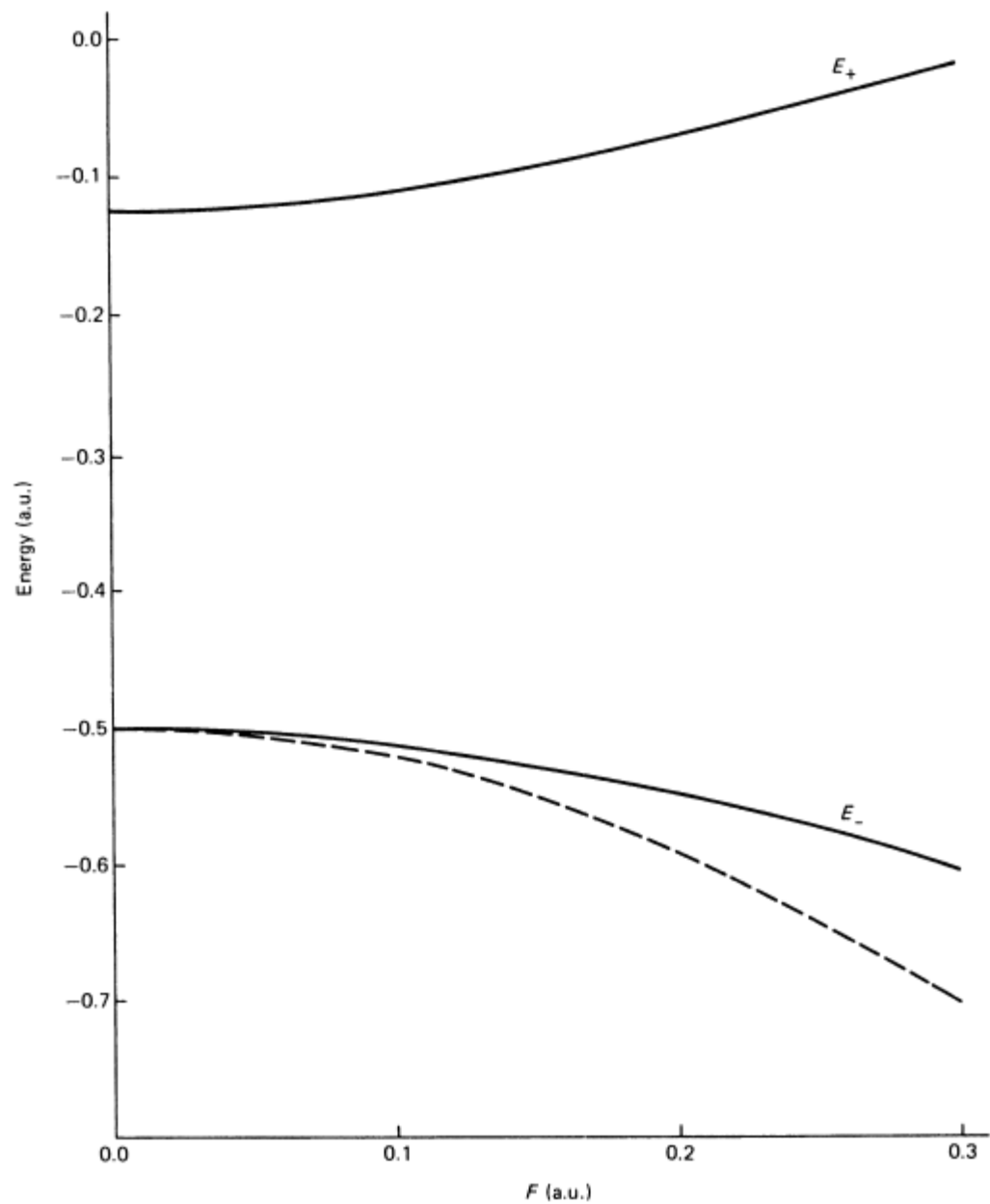


C9930, 3. přednáška, 17. 3. 2020

# Od variační metody k metodě EHT

Literatura: John P. Löwe, Quantum Chemistry

- Kapitola 7: část 7-4 (dokončení)
- Kapitola 8: část 8-13
- Kapitola 10: část 10-1



**Figure 7-3** ► Average energies for a hydrogen atom in a uniform electric field of strength  $F$  as given by a linear variation calculation using a  $1s, 2p_z$  basis. (---) Results from accurate calculations.

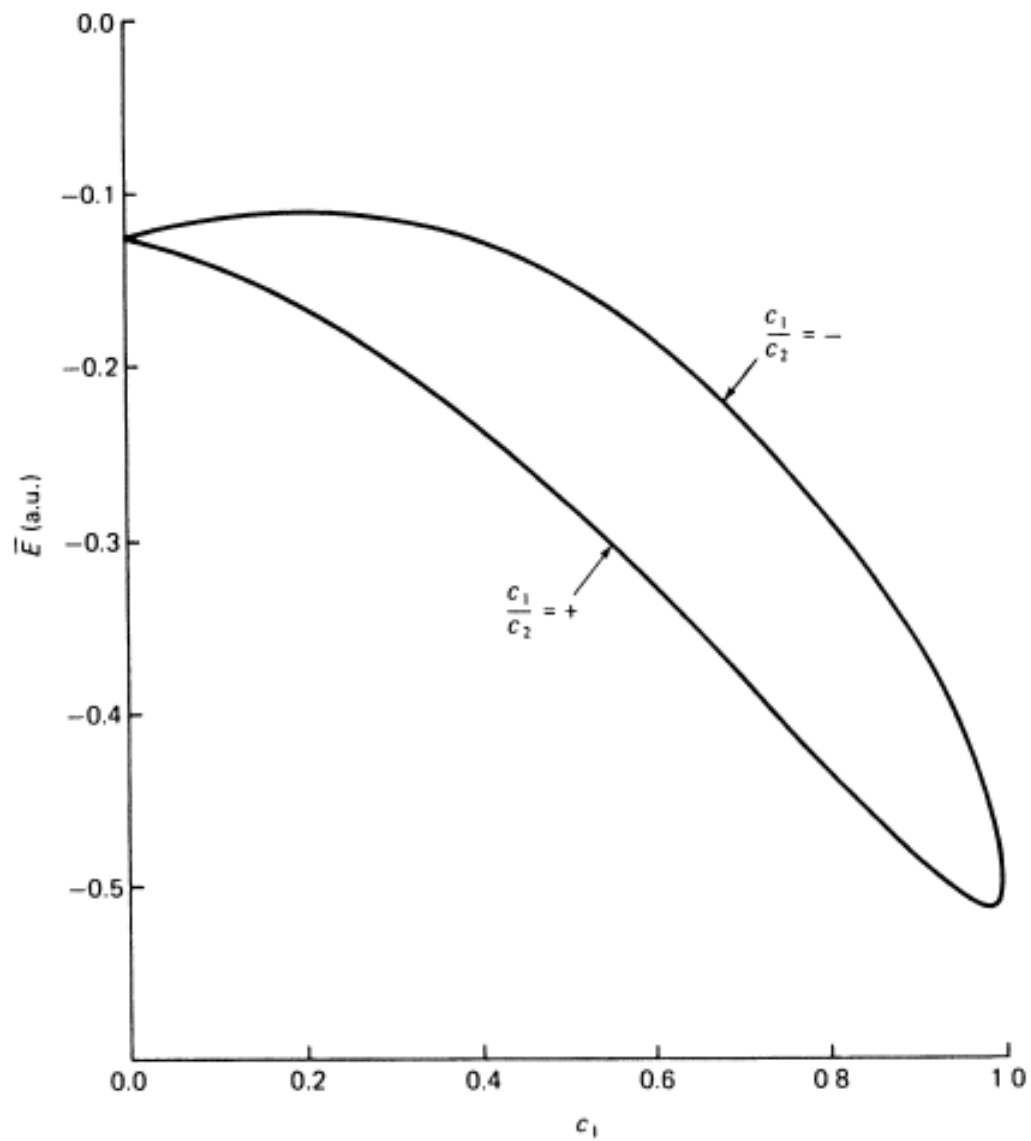
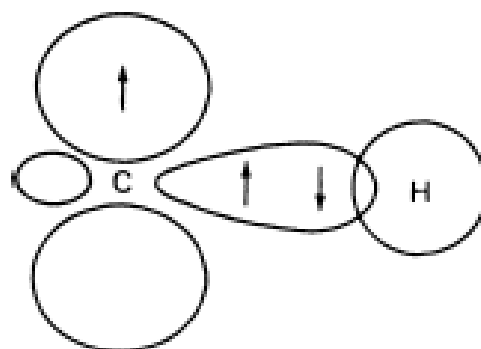
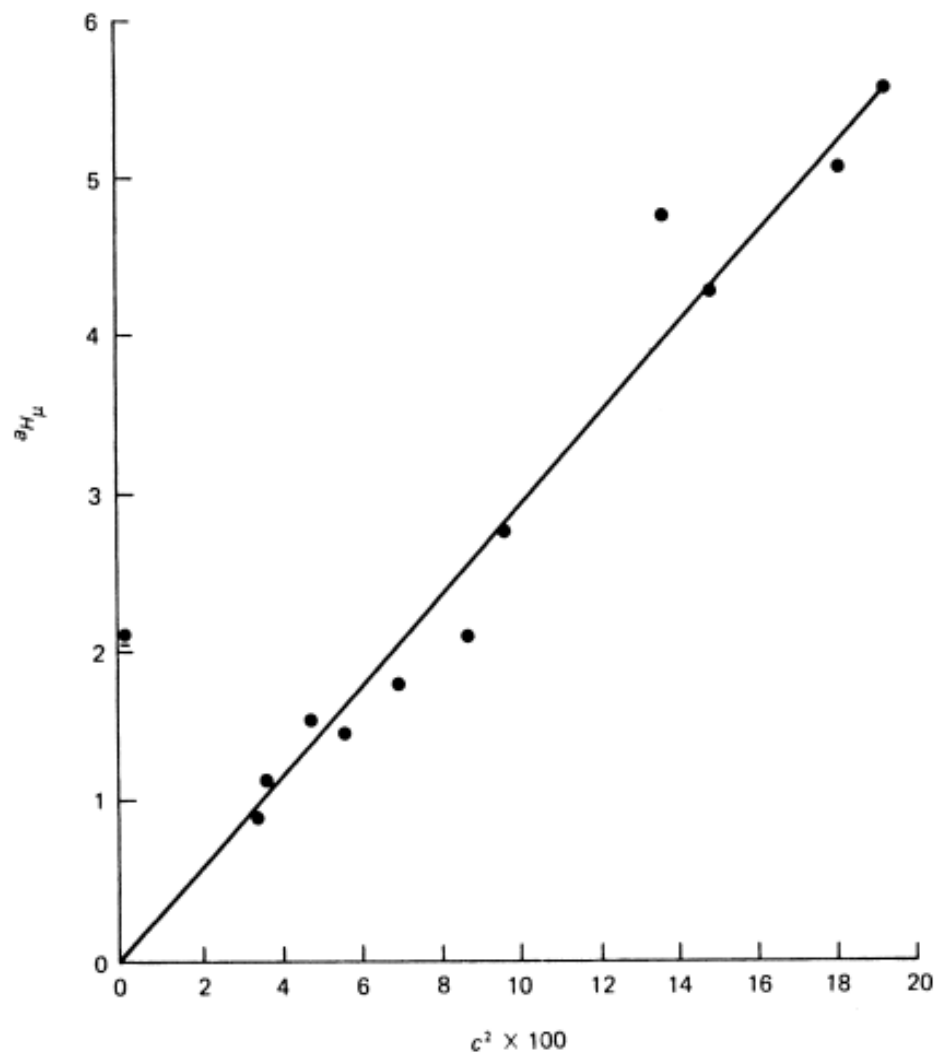


Figure 7-4 ►  $\bar{E}$  versus  $c_1$  for a hydrogen atom in a uniform electric field of strength 0.1 a.u.



**Figure 8-17** ► The unpaired  $\pi$ -spin density at carbon repels both  $\sigma$  electrons in the C–H bond region, but does not repel them equally. As a result, slight spin imbalance due to  $\sigma$  electrons occurs at the proton.



**Figure 8-18** ► ESR splitting constants  $a_{H\mu}$  in gauss versus HMO unpaired spin densities. The systems are fused ring alternant hydrocarbon radical anions (naphthalene, anthracene, tetracene, pyrene). The underlined point is thought to result from negative spin density. (Data from Streitwieser [7].)