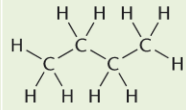
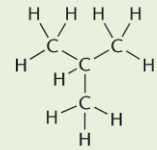
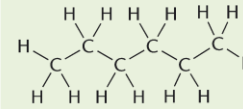
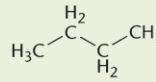
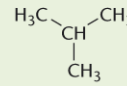
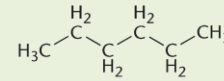
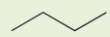
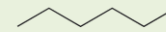
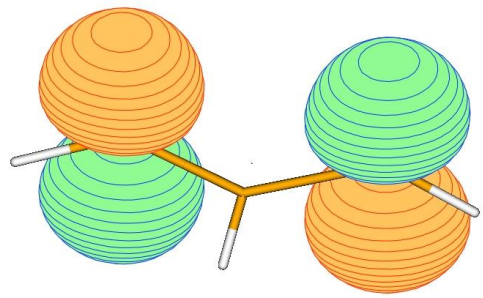
RAKENNEKAAVAT

Palautetaan mieleen orgaanisen molekyylin eri esitystavat.

Hiilivedyn nimi	butaani	2-metyylipropaani	heksaani
Molekyylikaava	C_4H_{10}	C_4H_{10}	C_6H_{14}
Rakennekaava **eli sidosviivakaava**			
Tiivistetty rakennekaava			
Viivakaava			

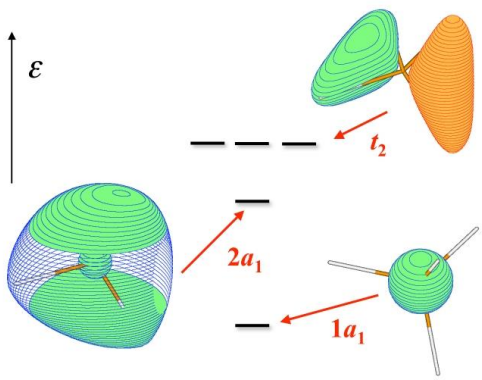
Molekyylimallinnus

Molekyylimallinnuksella tarkoitetaan yleisesti erilaisia teoreettisia ja laskennallisia menetelmiä, joilla pyritään mallintamaan molekyylien rakennetta ja käyttäytymistä. Molekyylimallinnusta käytetään laskennallisessa kemiassa ja biologiassa, materiaalitutkimuksessa ja lääkeainesuunnittelussa.



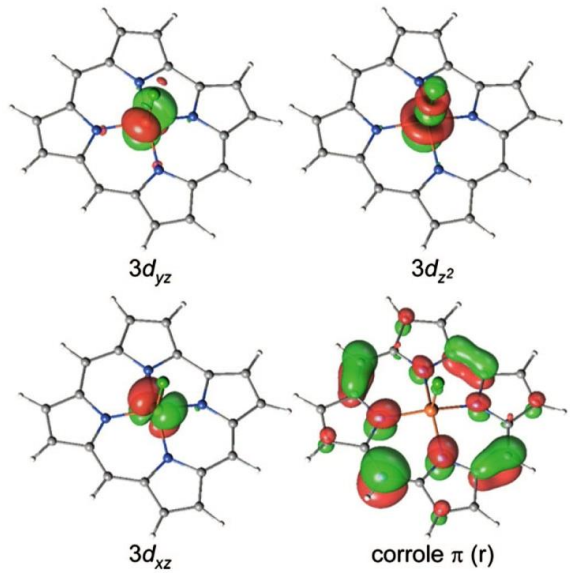
Canonical Hartree–Fock orbitals

- The canonical Hartree–Fock equations read: $\hat{F}\varphi_k = \varepsilon_k \varphi_k$



- By choosing the orbitals such that $\boldsymbol{\lambda}$ is diagonal, we obtain orbital energies ε_k as eigenvalues of the Fock operator.
- Note that canonical orbitals may look different from what you may have expected. The figure shows canonical MOs of methane, for example.

Ground-state MOs: Fe(IV)(corrolato)Cl



Anharmonic constants $\omega_e x_e$ of BH, CO, N_2, HF, and F_2 (cm^{-1})