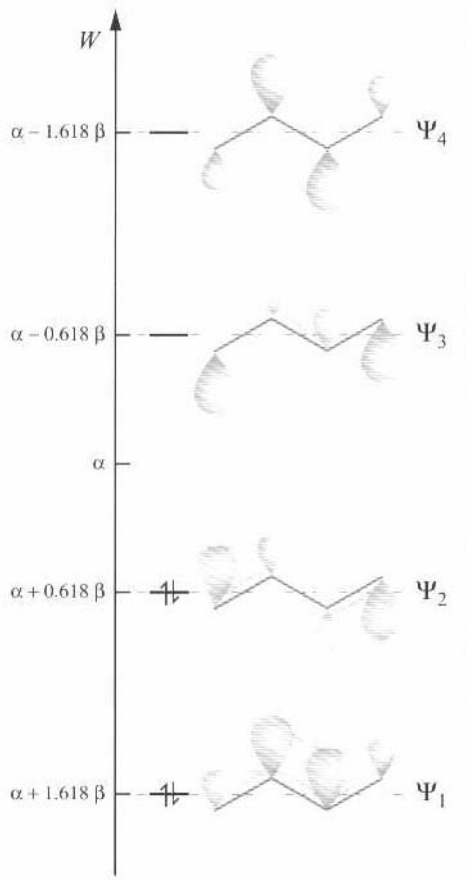
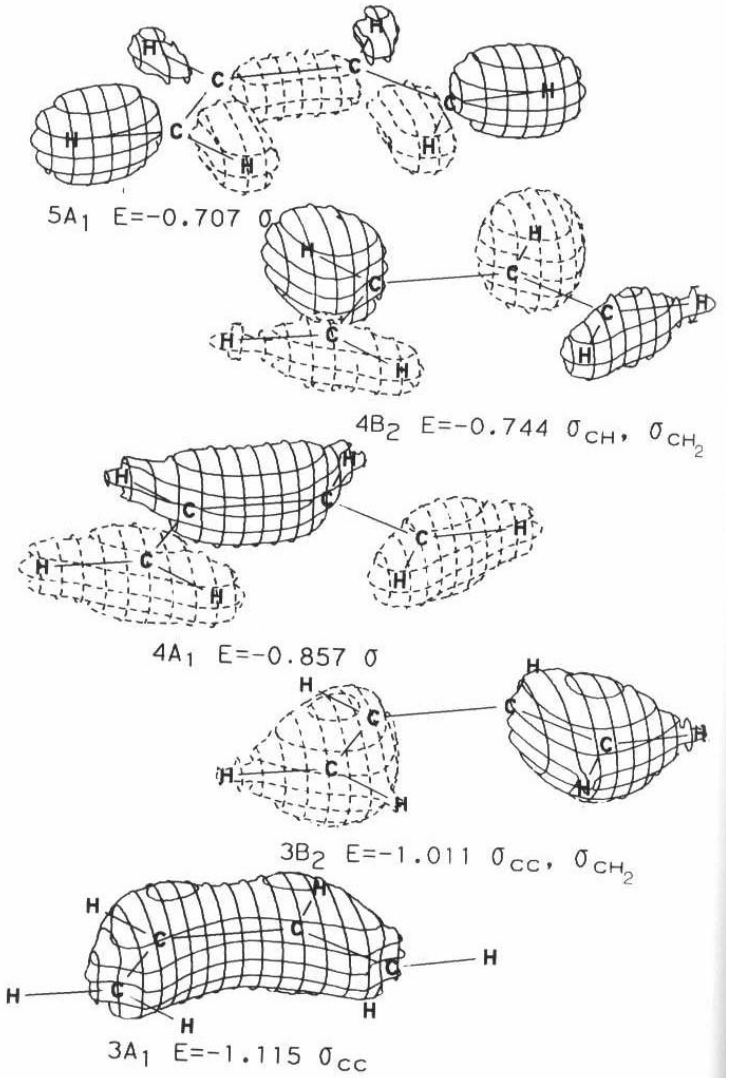
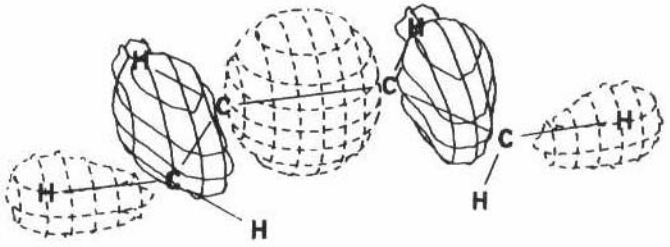


Figure 16: Result of the HMO calculation for buta-1,3-diene: energy levels and sketch of the wave functions of the π-MOs. The occupation of the energy levels is shown for the ground state.

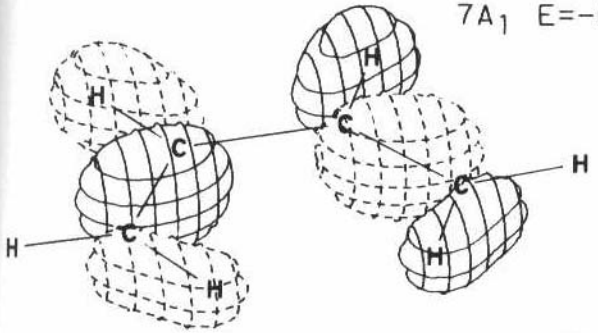
66. 1,3-Butadiene, Cisoid

Symmetry: C_{2v}

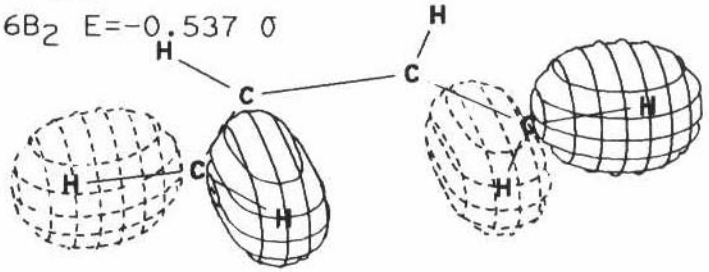




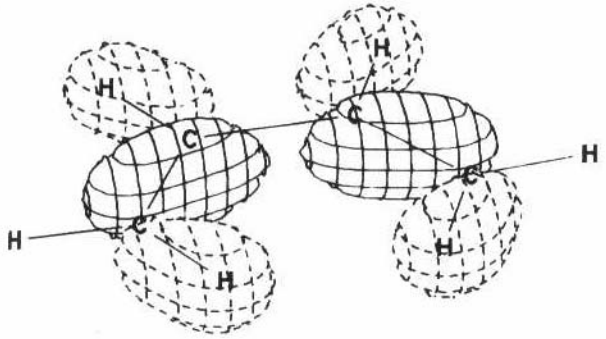
$7A_1$ E=-0.526 σ



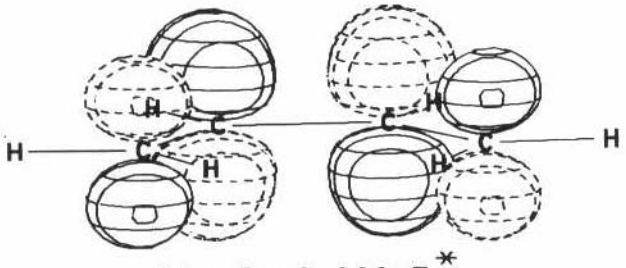
$6B_2$ E=-0.537 σ



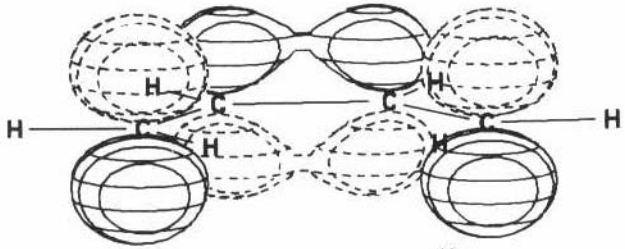
$5B_2$ E=-0.602 π'_{CH_2}



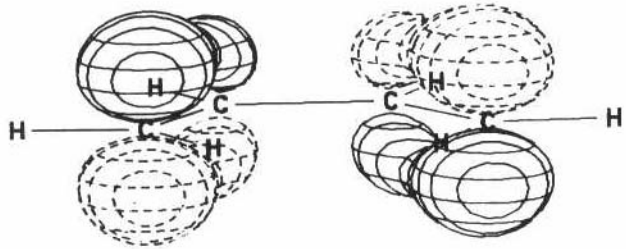
$6A_1$ E=-0.629 σ



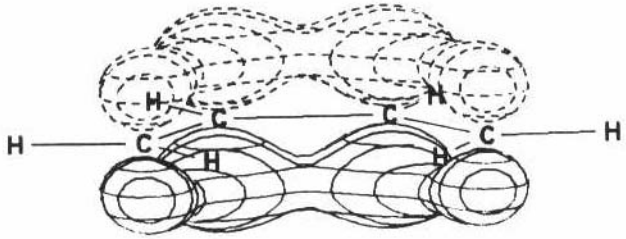
$2A_2$ E= 0.289 π^*_4



$2B_1$ E= 0.120 π^*_3



$1A_2$ E=-0.354 π_2



$1B_1$ E=-0.477 π_1

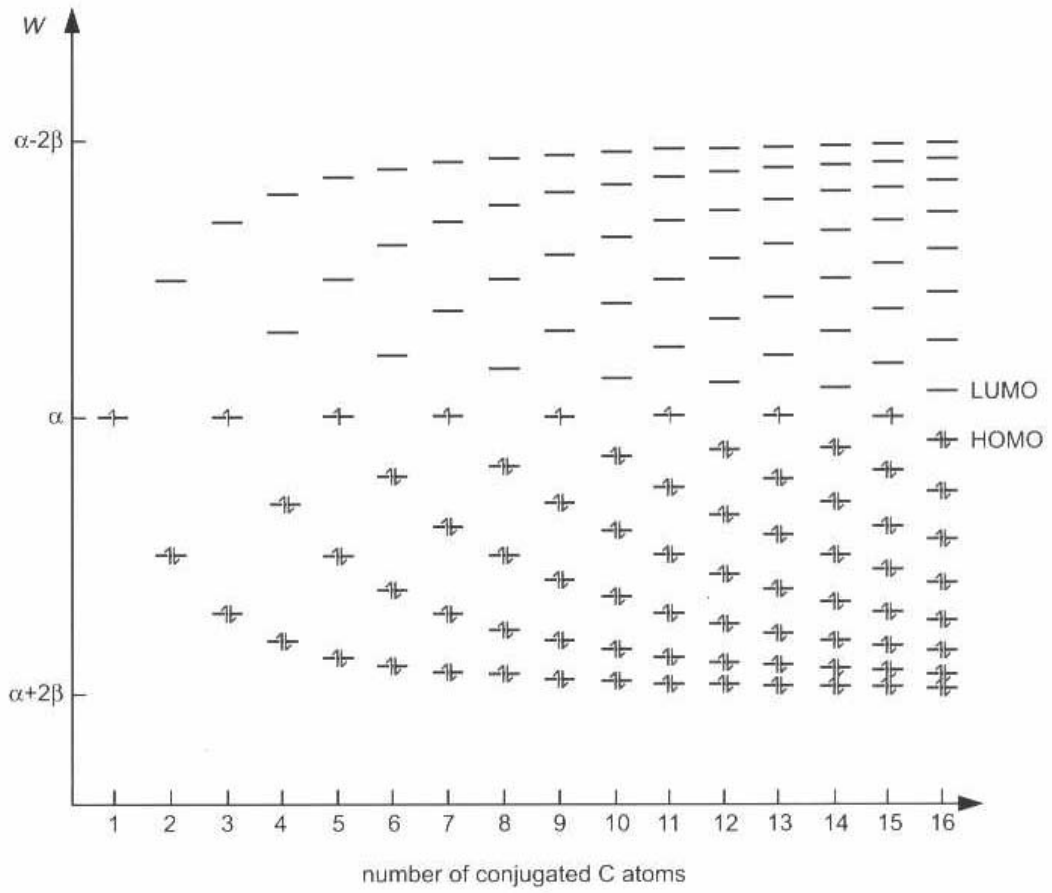
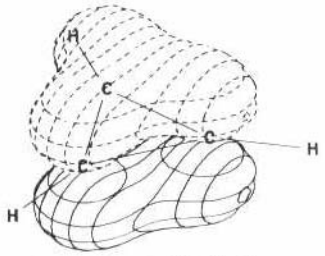


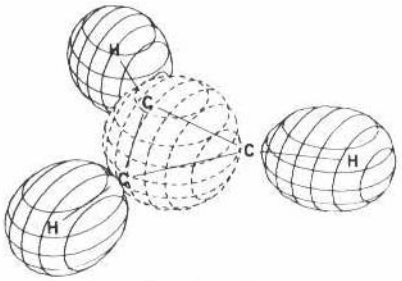
Figure 17: Energy levels and electron occupation for conjugated hydrocarbon with unbranched chain structures of one to 22 C atoms as calculated by the HMO theory. The system with one C atom represents a sp^2-hybridized CH_3 radical.

37. Cyclopropenium Cation

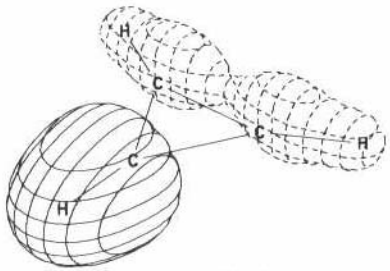
Symmetry: D_{3h}



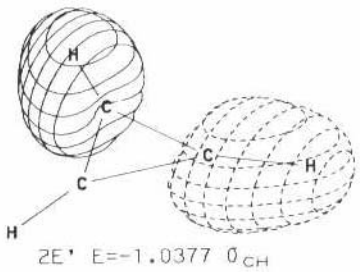
$1A_2''$ E=-0.7196 π_{CC}



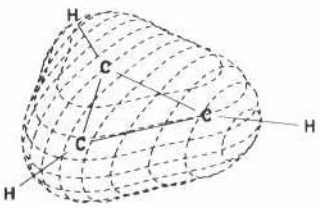
$3A_1'$ E=-0.8111 σ_{CC}, σ_{CH}



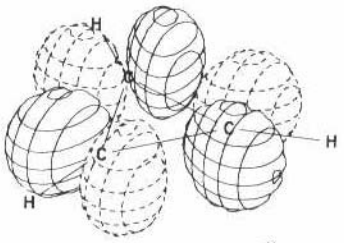
$2E'$ E=-1.0377 σ_{CH}



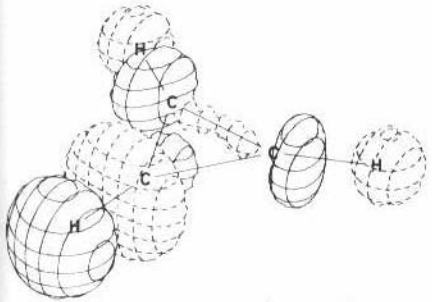
$2E'$ E=-1.0377 σ_{CH}



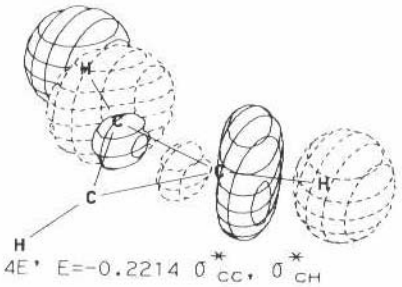
$2A_1'$ E=-1.5934 σ_{CC}



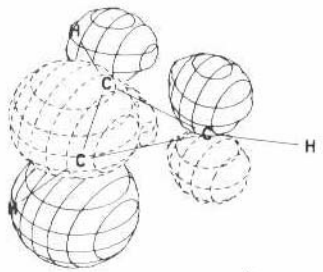
$1A_2'$ E=-0.1680 σ^*_{CC}



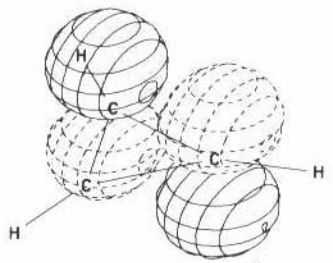
$4E'$ E=-0.2214 σ^*_{CC}, σ^*_{CH}



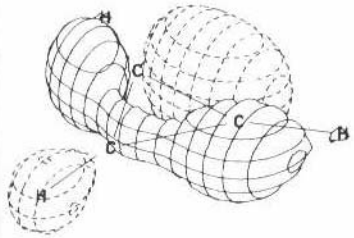
$4E'$ E=-0.2214 σ^*_{CC}, σ^*_{CH}



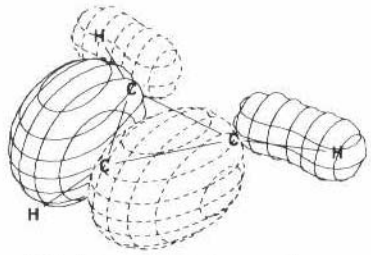
$1E''$ E=-0.2445 π^*_{CC}



$1E''$ E=-0.2445 π^*_{CC}



$3E'$ E=-0.6641 σ_{CC}, σ_{CH}



$3E'$ E=-0.6641 σ_{CC}, σ_{CH}