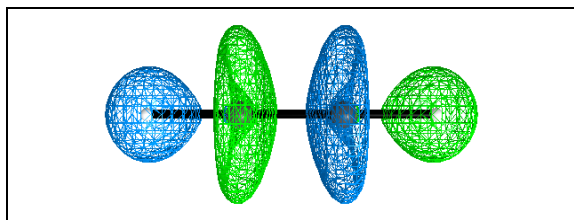
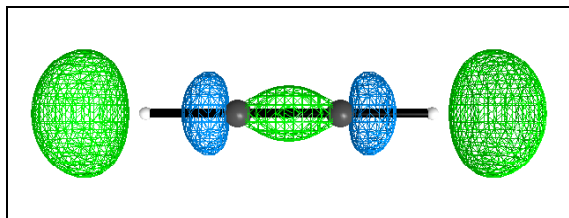


MOs of HCCH

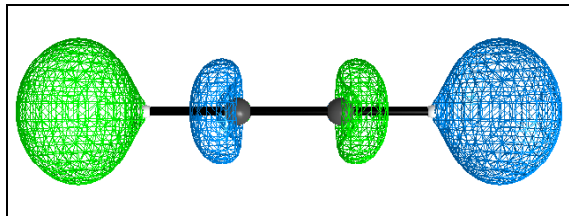
0.625



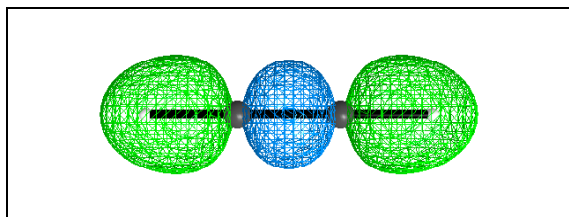
0.298



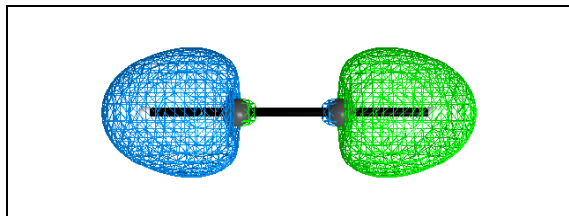
0.253



-0.673



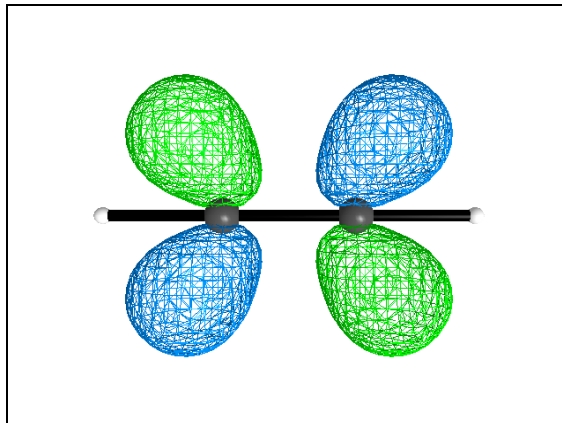
-0.760



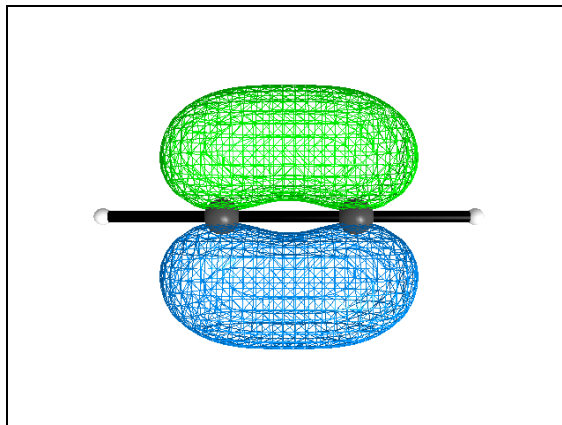
RHF/6-31G* level

E's in AU (Hartrees); 1 H = 627.5 kcal/mol
rCC = 1.185; rCH = 1.057

0.222(x2)



-0.405(x2)



-1.025

