

Localization of the filled and virtual orbitals in the nucleotide bases. Cizek, J.; Foerner, W.; Ladik, J.

Abstract

Both Boys (B) and Edminston-Ruedenberg (ER) localization procedures of the ab initio canonical orbitals were performed for the 4 nucleotide bases (cytosine, uracil, adenine and guanine). The results obtained for both σ - π sepn. and by treating all electrons together show very good localization for all electrons (1-center lone-pairs and 2-center localized orbitals even for π -electrons), and rather good localization for the virtuals applying both B and ER criteria. The results of the 2 methods are essentially identical.