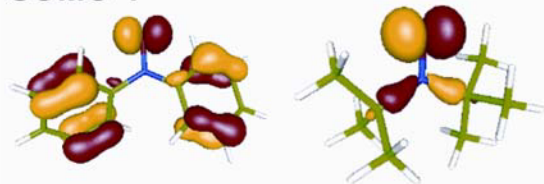


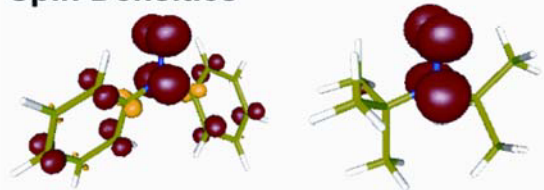
## SOMO's



## SOMO-1



## Spin Densities



**Figure 6.** The semioccupied molecular orbitals (SOMOs), the doubly occupied SOMO-1 orbitals, and the spin densities of the DPNO (left) and DTBNO radicals (right). The SOMOs give an impression of the delocalization of the unpaired electron in these systems. The dominating  $\Delta g_{xx}$  shift is mainly the result of an electronic excitation from the SOMO-1 level to the SOMO orbitals. Reproduced with permission from [133]. Copyright © 2006, American Chemical Society.