

# The Molecular orbitals of the open-shell system of the methyl free radical as determined by dual space analysis

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Dual Space Analysis (DSA), using momentum and orbital electron density distributions spanning both the core and valence spaces, of the simplest of organic radicals, methyl free radical -  $\text{CH}_3^\bullet$ , have been calculated, employing *ab initio* (HF - UHF and ROHF, and hybrid DFT - B3LYP) techniques with the DGauss (DFT Orbital) triple-zeta basis set (TZVP).

Comparisons are drawn between  $\text{CH}_3^\bullet$ , and other small related species, such as:  $\text{CH}_4$ ,  $\text{CH}_3^+$  and  $\text{CH}_3^-$ , as well as  $\text{NH}_3$  and  $\text{NH}_3^+$ .