Carbon, M = (CCSD, aug-cc-pVTZ)

Oxygen, M = (CCSD, aug-cc-pVTZ)

$E_c(\bar{\rho}_1^M) \approx -138.126\,\mathrm{mE_h}$ (integrated)
$\approx -138.076\,\mathrm{mE_h}$ (direct)

$E_c(\bar{\rho}_1^M) \approx -221.285\,\mathrm{mE_h}$ (integrated)
$\approx -221.143\,\mathrm{mE_h}$ (direct)

PSVR

PSVR

$\mathcal{W}_\lambda(\bar{\rho}_\lambda^M) - \mathcal{W}_0(\bar{\rho}_0^M)\,/\,\mathrm{E_h}$

0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
−0.35
−0.40
−0.45

Totally symmetric ensemble density
Degenerate pure-state density

$\|\bar{\rho}_\lambda^M - \bar{\rho}_1^M\|_2$

10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}

[He] $2s^2 2p^2$ config., Hartree–Fock reference

[He] $2s^2 2p^4$ config., Hartree–Fock reference

HOMO–LUMO gap / $\mathrm{E_h}$

0.0
0.2
0.4
0.6
0.8

$\beta 2s^{\mathrm{occ}} - \beta 2p^{\mathrm{vir}}$

$\alpha 2p^{\mathrm{occ}} - \alpha 2p^{\mathrm{vir}}$

$\alpha 2p^{\mathrm{occ}} - \alpha 3s^{\mathrm{vir}}$

$\beta 2p^{\mathrm{occ}} - \beta 2p^{\mathrm{vir}}$

0.0 0.2 0.4 0.6 0.8 1.0

λ

premature

premature

α HOMO–LUMO degeneracy

β HOMO–LUMO degeneracy