$\Delta\rho_1{}^\ominus$

Δq_1 = 0.271 a.u.

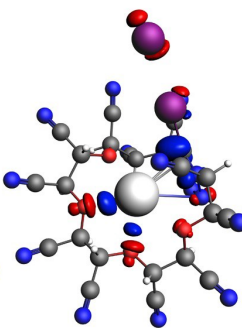$\Delta E_{oi,1}$ = −3.41 kcal mol⁻¹

$\Delta\rho_2{}^\ominus$
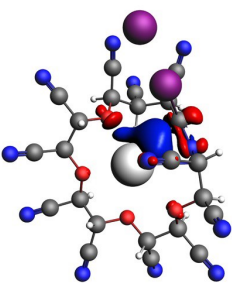
Δq_2 = 0.123 a.u.

$\Delta E_{oi,2}$ = −2.83 kcal mol⁻¹

$\Delta\rho_3{}^\ominus$

Δq_3 = 0.107 a.u.

$\Delta E_{oi,3}$ = −2.38 kcal mol⁻¹

$\Delta\rho_4{}^*$
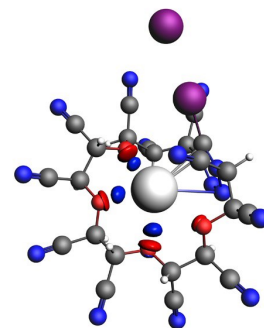
Δq_4 = 0.098 a.u.

$\Delta E_{oi,4}$ = −2.56 kcal mol⁻¹

$\Delta\rho_5{}^*$
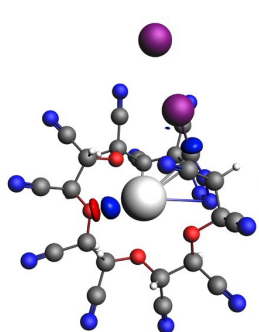
Δq_5 = 0.094 a.u.

$\Delta E_{oi,5}$ = −2.06 kcal mol⁻¹

$\Delta\rho_6{}^\ominus$
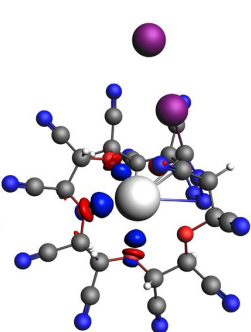
Δq_6 = 0.087 a.u.

$\Delta E_{oi,6}$ = −2.04 kcal mol⁻¹

$\Delta\rho_7{}^\ominus$
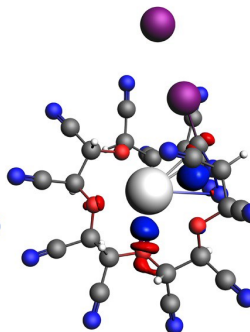
Δq_7 = 0.080 a.u.

$\Delta E_{oi,7}$ = −1.65 kcal mol⁻¹

$\Delta\rho_8{}^\ominus$
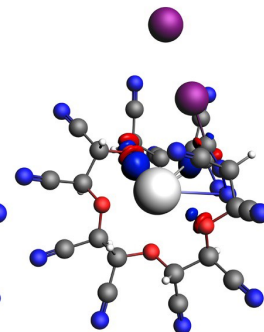
Δq_8 = 0.076 a.u.

$\Delta E_{oi,8}$ = −1.79 kcal mol⁻¹

$\Delta\rho_9{}^\ominus$
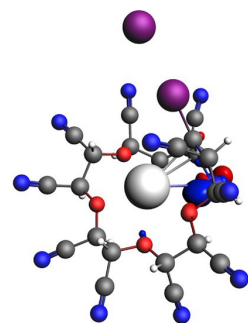
Δq_9 = 0.063 a.u.

$\Delta E_{oi,9}$ = −1.09 kcal mol⁻¹

$\Delta\rho_{11}{}^\ominus$
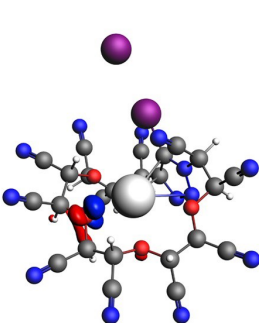
Δq_{11} = 0.055 a.u.

$\Delta E_{oi,11}$ = −1.03 kcal mol⁻¹

$\Delta\rho_{12}{}^\sigma$
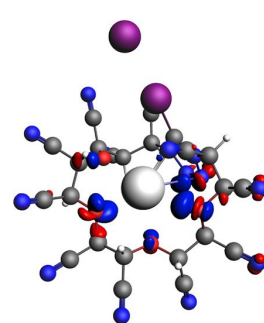
Δq_{12} = 0.051 a.u.

$\Delta E_{oi,12}$ = −0.90 kcal mol⁻¹