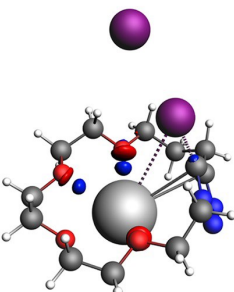


$\Delta\rho_1^*$

$\Delta q_1 = 0.132$ a.u.

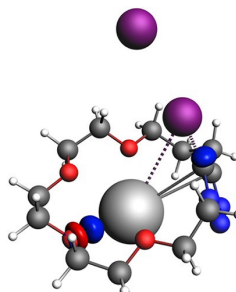
$\Delta E_{oi,1} = -2.62$ kcal mol⁻¹



$\Delta\rho_2^*$

$\Delta q_2 = 0.123$ a.u.

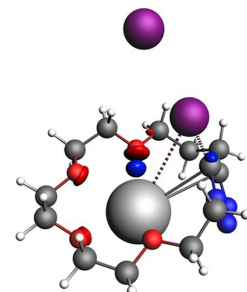
$\Delta E_{oi,2} = -2.63$ kcal mol⁻¹



$\Delta\rho_3^*$

$\Delta q_1 = 0.119$ a.u.

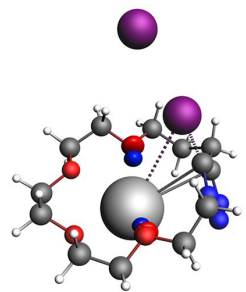
$\Delta E_{oi,3} = -2.23$ kcal mol⁻¹



$\Delta\rho_4^*$

$\Delta q_4 = 0.112$ a.u.

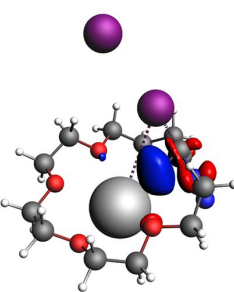
$\Delta E_{oi,4} = -2.27$ kcal mol⁻¹



$\Delta\rho_5^*$

$\Delta q_5 = 0.100$ a.u.

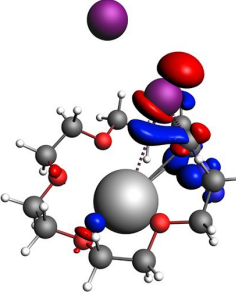
$\Delta E_{oi,5} = -1.95$ kcal mol⁻¹



$\Delta\rho_6^\ominus$

$\Delta q_6 = 0.091$ a.u.

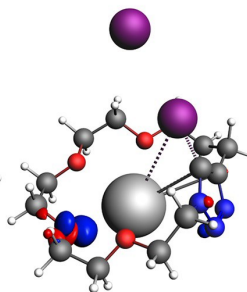
$\Delta E_{oi,6} = -1.73$ kcal mol⁻¹



$\Delta\rho_7^\ominus$

$\Delta q_7 = 0.080$ a.u.

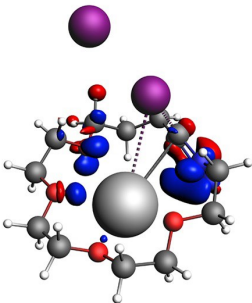
$\Delta E_{oi,7} = -1.24$ kcal mol⁻¹



$\Delta\rho_8^\ominus$

$\Delta q_8 = 0.060$ a.u.

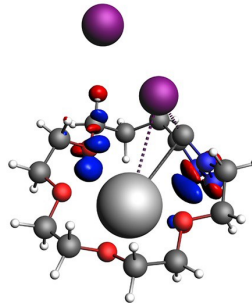
$\Delta E_{oi,8} = -0.90$ kcal mol⁻¹



$\Delta\rho_9^\ominus$

$\Delta q_9 = 0.057$ a.u.

$\Delta E_{oi,9} = -0.83$ kcal mol⁻¹



$\Delta\rho_{10}^\ominus$

$\Delta q_{10} = 0.054$ a.u.

$\Delta E_{oi,10} = -0.79$ kcal mol⁻¹