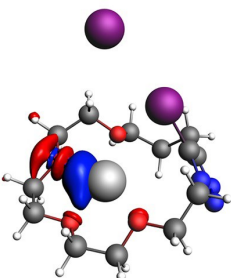


$\Delta\rho_1^*$

$\Delta q_1 = 0.174 \text{ a.u.}$

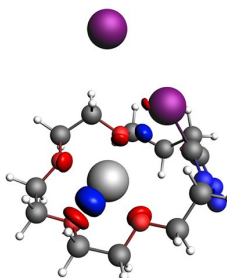
$\Delta E_{oi,1} = -6.69 \text{ kcal mol}^{-1}$



$\Delta\rho_2^*$

$\Delta q_2 = 0.168 \text{ a.u.}$

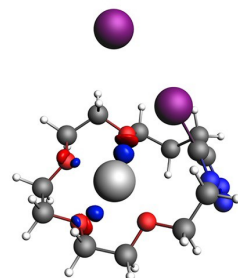
$\Delta E_{oi,2} = -6.59 \text{ kcal mol}^{-1}$



$\Delta\rho_3^*$

$\Delta q_3 = 0.145 \text{ a.u.}$

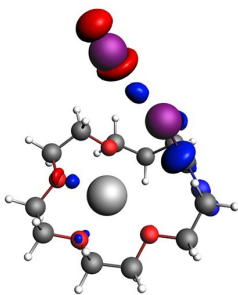
$\Delta E_{oi,3} = -4.10 \text{ kcal mol}^{-1}$



$\Delta\rho_4^*$

$\Delta q_4 = 0.118 \text{ a.u.}$

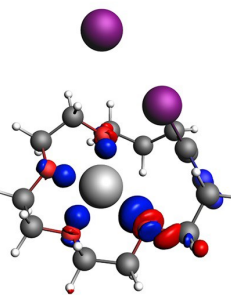
$\Delta E_{oi,4} = -2.82 \text{ kcal mol}^{-1}$



$\Delta\rho_5^\ominus$

$\Delta q_5 = 0.097 \text{ a.u.}$

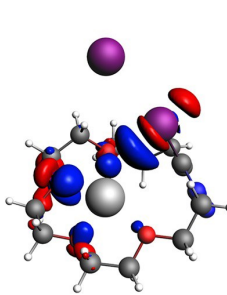
$\Delta E_{oi,5} = -1.47 \text{ kcal mol}^{-1}$



$\Delta\rho_6^\ominus$

$\Delta q_6 = 0.083 \text{ a.u.}$

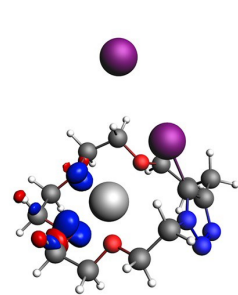
$\Delta E_{oi,6} = -1.99 \text{ kcal mol}^{-1}$



$\Delta\rho_7^\text{d}$

$\Delta q_7 = 0.074 \text{ a.u.}$

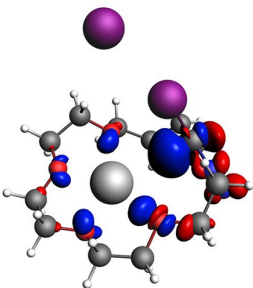
$\Delta E_{oi,7} = -1.58 \text{ kcal mol}^{-1}$



$\Delta\rho_8^\ominus$

$\Delta q_8 = 0.072 \text{ a.u.}$

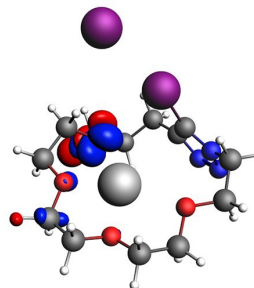
$\Delta E_{oi,8} = -1.58 \text{ kcal mol}^{-1}$



$\Delta\rho_9^\text{d}$

$\Delta q_9 = 0.063 \text{ a.u.}$

$\Delta E_{oi,9} = -1.12 \text{ kcal mol}^{-1}$



$\Delta\rho_{10}^\text{b}$

$\Delta q_{10} = 0.051 \text{ a.u.}$

$\Delta E_{oi,10} = -0.88 \text{ kcal mol}^{-1}$