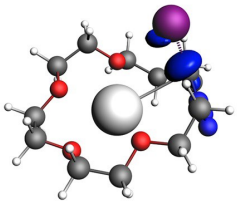
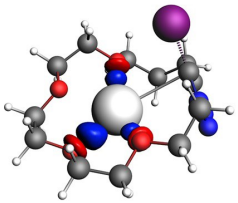
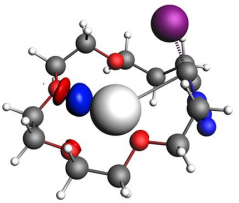
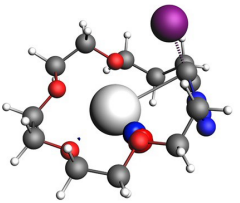








$\Delta\rho_2$*

Δq_2 = 0.126 a.u.

$\Delta E_{oi,2}$ = –1.89 kcal mol^{-1}

$\Delta\rho_3$*

Δq_3 = 0.107 a.u.

$\Delta E_{oi,3}$ = –2.86 kcal mol^{-1}

$\Delta\rho_4$*

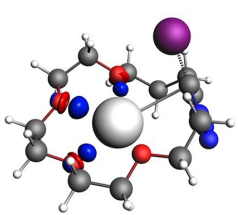
Δq_4 = 0.106 a.u.

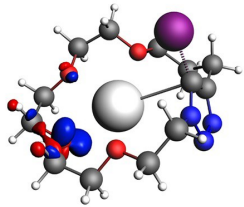
$\Delta E_{oi,4}$ = –2.77 kcal mol^{-1}

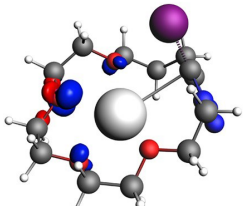
$\Delta\rho_5$*

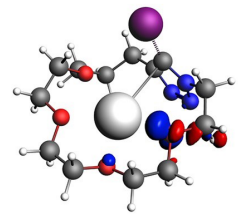
Δq_5 = 0.090 a.u.

$\Delta E_{oi,5}$ = –2.01 kcal mol^{-1}









$\Delta\rho_6$*

Δq_6 = 0.087 a.u.

$\Delta E_{oi,6}$ = –2.20 kcal mol^{-1}

$\Delta\rho_8^{\ominus}$

Δq_8 = 0.062 a.u.

$\Delta E_{oi,8}$ = –1.05 kcal mol^{-1}

$\Delta\rho_9^{\ominus}$

Δq_9 = 0.057 a.u.

$\Delta E_{oi,9}$ = –0.97 kcal mol^{-1}

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

Δq_{10} = 0.051 a.u.

$\Delta E_{oi,10}$ = –0.74 kcal mol^{-1}