# NEW ENERGY PARTITIONING SCHEME BASED ON THE SELF-CONSISTENT CONFIGURATION METHOD FOR SUBSYSTEMS

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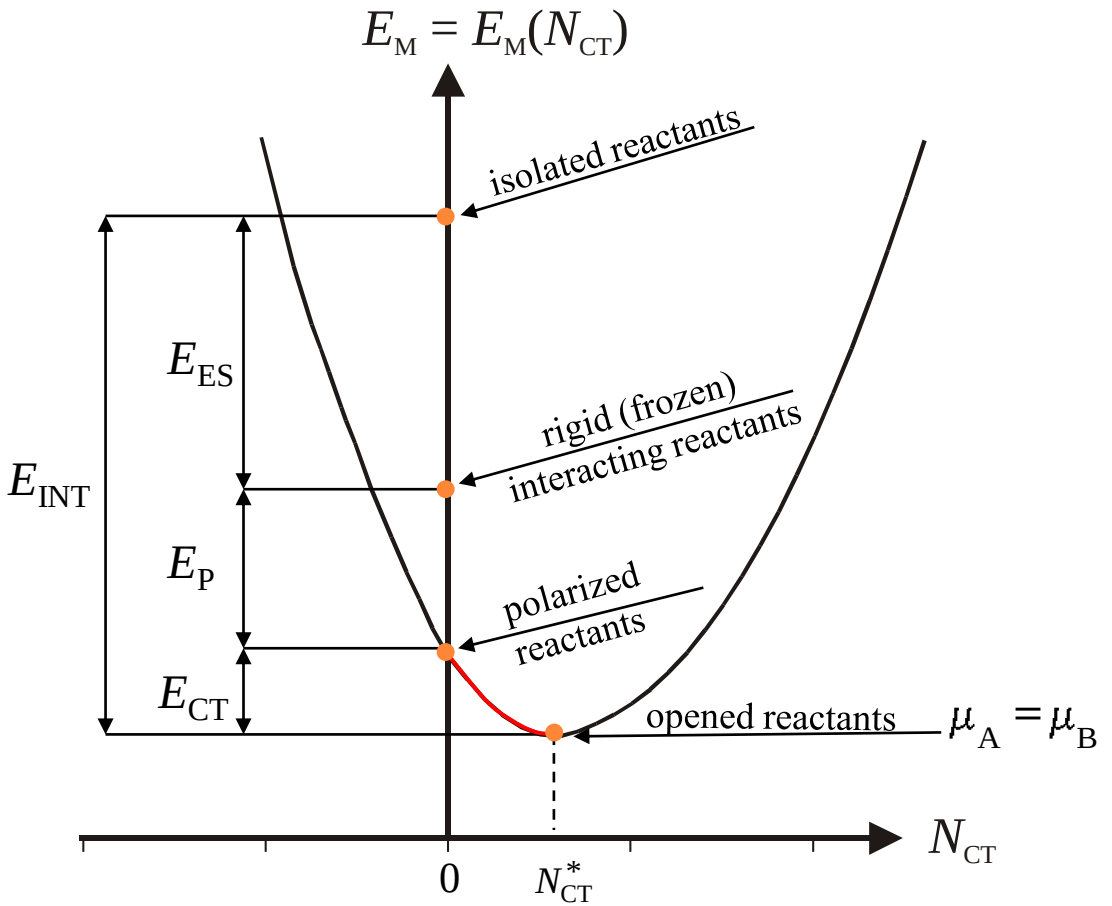
# Components of interaction energy

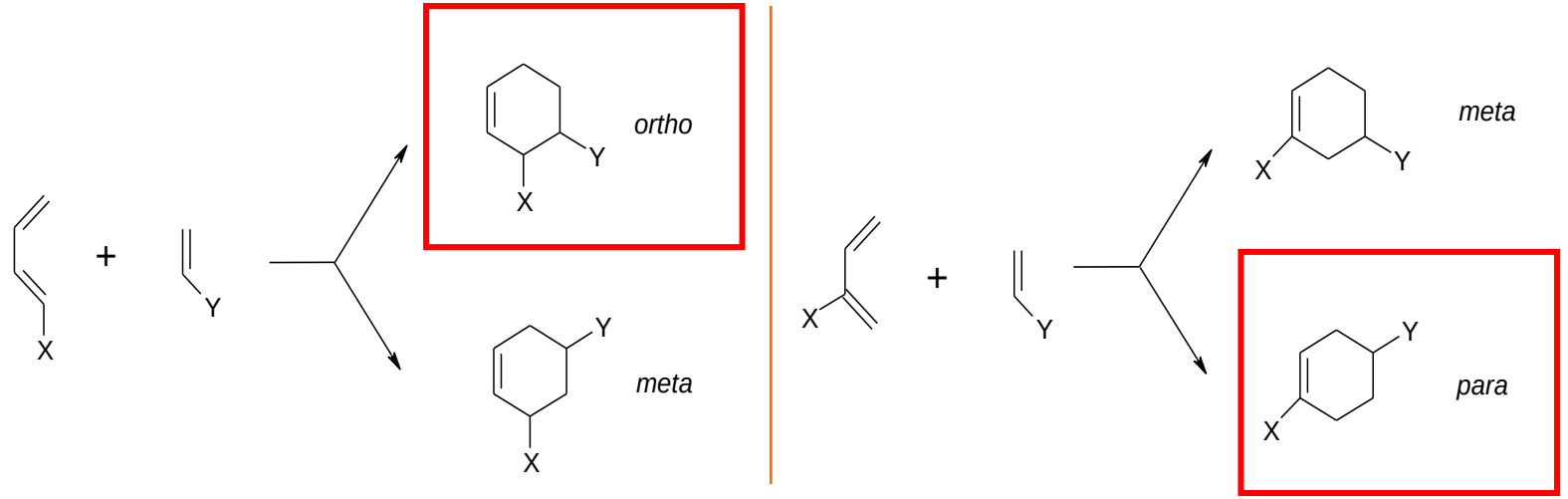



$$\mu_A \equiv (\partial E_M / \partial N_A)_{v,N_B} = \mu_A(\vec{r}) \equiv [\delta E_M / \delta \rho_A(\vec{r})]_{v,N_B}$$

$$\mu_B \equiv (\partial E_M / \partial N_B)_{v,N_A} = \mu_B(\vec{r}) \equiv [\delta E_M / \delta \rho_B(\vec{r})]_{v,N_A}$$

$$\mu_A \neq \mu_B$$

# Model systems: Diels-Alder Reaction




X = H, CN, Cl, F, $CH_3$, OH and $NH_2$

Y = H, Cl, F, $CH_3$ and OH

# Dependence of $E_{CT}$ on $N_{CT}$ for different cycloadducts