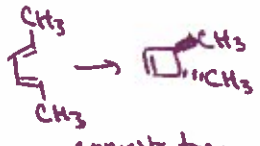
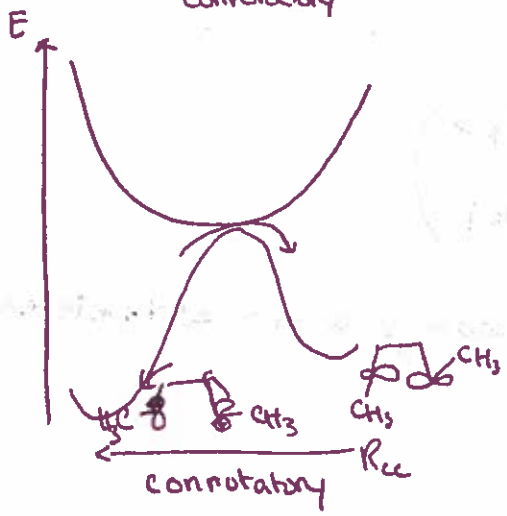
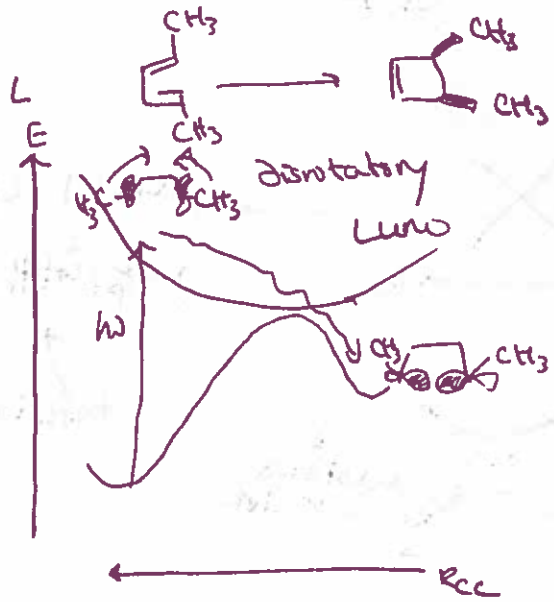
Hexatriene: $4n\ \pi e^-$, $n=1$] last time

Heat:



conrotatory



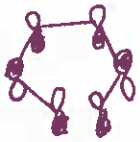


Homework: octatriene, $4n+2\ \pi e^-$, $n=1$

Heat?
Light?

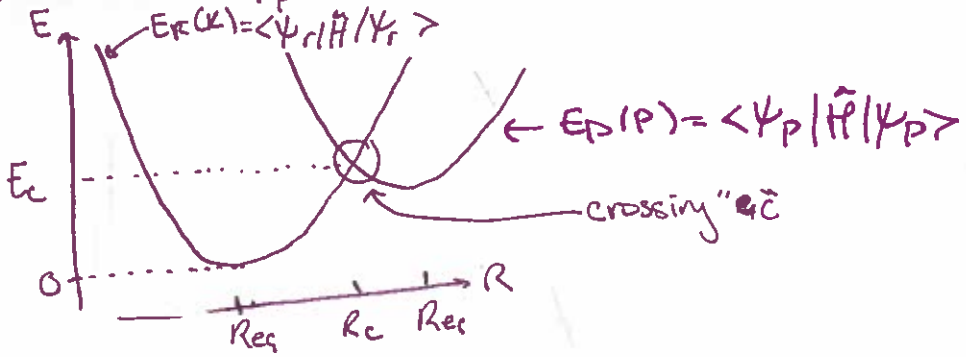
One more π bond ⟶ one ~~node~~ more node
⟶ Flip the phase of the Homo and Lumo

Homo



Is it a coincidence the energy looks like  ? Answer, No

Consider reactant energy $E_R(R)$ & wavefunction ψ_r, and a product energy $E_p(R)$ & wavefunction ψ_p



Near the crossing,

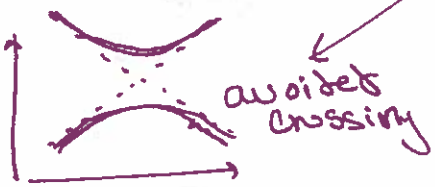
$E_r \approx E_c + m_r (R - R_c)$ (m_r: slope, > 0)

$E_p(R) \approx E_c + m_p (R - R_c)$ (m_p: slope, < 0)

Zoom in

$$\begin{pmatrix} E_r(R) & \langle \psi_r | \hat{H} | \psi_p \rangle \\ \langle \psi_p | \hat{H} | \psi_r \rangle & E_p(R) \end{pmatrix}$$

there is almost always a $\neq 0$ matrix element



True Core