

Hückel

$$\text{Ethylene: } 2 \cdot \underbrace{(d+m)}_{\text{electron}} = 2d + 2m$$

d = energy of a "p" atomic orbital

m = stabilization of the MO (negative)

$\beta \rightarrow$ found empirically

barriere of isomerization = 65 kcal mol⁻¹

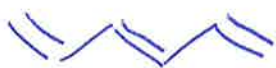
$$\beta \approx -32 \text{ kcal mol}^{-1}$$

$$\text{cyclobutadiene} = 2d + 4m + 2d = 4d + 4m$$

$$2 \text{ ethylene} = 4d + 4m$$

} 0

Hückel:



$$E_1 = \alpha + 2\gamma \overbrace{\cos \frac{\pi}{7}}^{0.9}$$
$$= \alpha + 1.8\gamma$$

$$E_2 = \alpha + 2\gamma \cdot \overbrace{\cos \frac{2\pi}{7}}^{0.62}$$
$$= \alpha + 1.24\gamma$$

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$$E_0 = \alpha + 2\gamma \cdot \cos 0$$
$$= \alpha + 2\gamma$$

$$E_1 = \alpha + 2\gamma \cdot \underbrace{\cos \frac{2\pi}{6}}_{0.5}$$
$$= \alpha + \gamma$$