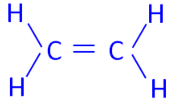
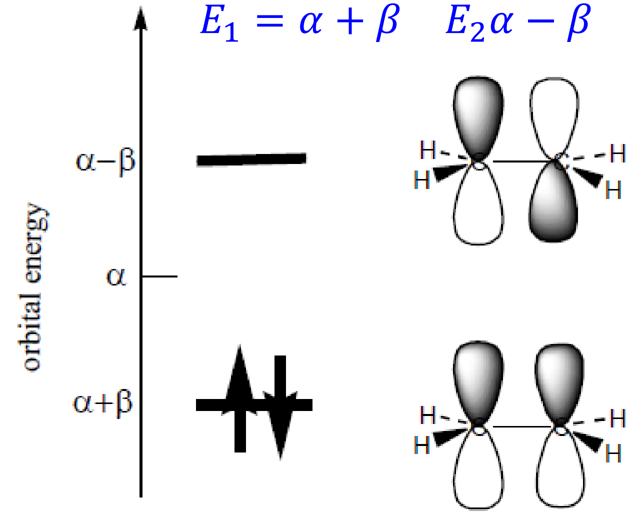
分子軌道

エチレン



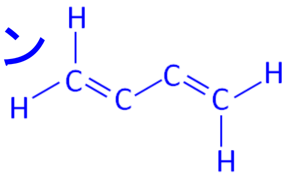


$E_1 = \alpha + \beta \quad E_2 \alpha - \beta$

$$\begin{vmatrix} \alpha - E & \beta \\ \beta & \alpha - E \end{vmatrix} = \begin{vmatrix} \frac{\alpha - E}{\beta} & 1 \\ 1 & \frac{\alpha - E}{\beta} \end{vmatrix} = \begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda \end{vmatrix} = 0$$

$\lambda^2 - 1 = 0$ より $\lambda = \pm 1$

ブタジエン



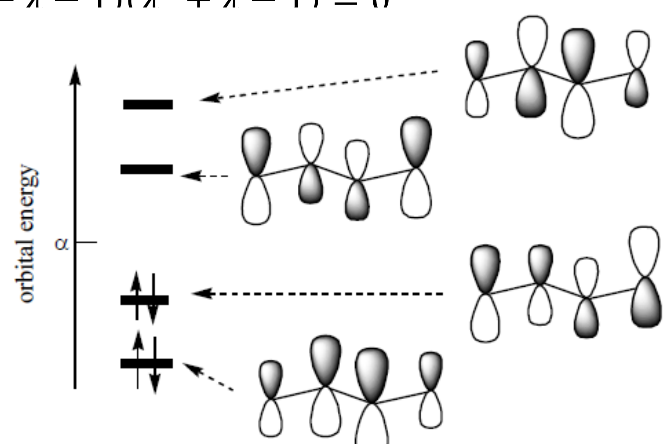
$$\begin{vmatrix} \alpha - E & \beta & 0 & 0 \\ \beta & \alpha - E & \beta & 0 \\ 0 & \beta & \alpha - E & \beta \\ 0 & 0 & \beta & \alpha - E \end{vmatrix} = \begin{vmatrix} \frac{\alpha - E}{\beta} & 1 & 0 & 0 \\ 1 & \frac{\alpha - E}{\beta} & 1 & 0 \\ 0 & 1 & \frac{\alpha - E}{\beta} & 1 \\ 0 & 0 & 1 & \frac{\alpha - E}{\beta} \end{vmatrix} = \begin{vmatrix} -\lambda & 1 & 0 & 0 \\ 1 & -\lambda & 1 & 0 \\ 0 & 1 & -\lambda & 1 \\ 0 & 0 & 1 & -\lambda \end{vmatrix} = 0$$

$$-\lambda \begin{vmatrix} -\lambda & 1 & 0 \\ 1 & -\lambda & 1 \\ 0 & 1 & -\lambda \end{vmatrix} - \begin{vmatrix} 1 & 0 & 0 \\ 1 & -\lambda & 1 \\ 0 & 1 & -\lambda \end{vmatrix} = \lambda(\lambda^3 - 2\lambda) - (\lambda^2 - 1) = (\lambda^2 - \lambda - 1)(\lambda^2 + \lambda - 1) = 0$$

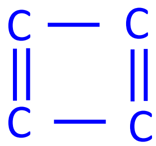
$$\lambda = \pm \frac{\sqrt{5} \pm 1}{2}$$

$E_1 = \alpha + \frac{\sqrt{5}+1}{2}\beta \quad E_2 = \alpha + \frac{\sqrt{5}-1}{2}\beta$

$E_3 = \alpha - \frac{\sqrt{5}-1}{2}\beta \quad E_4 = \alpha - \frac{\sqrt{5}+1}{2}\beta$



シクロブタジエン

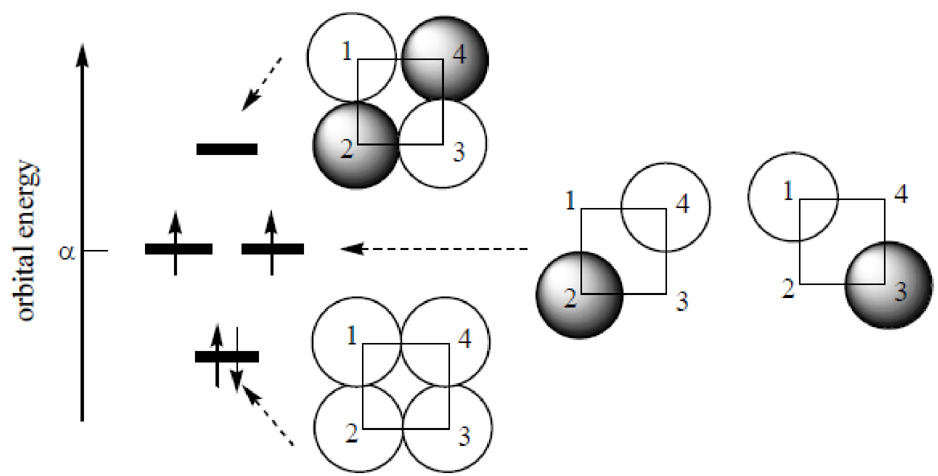


$$\begin{vmatrix} \alpha-E & \beta & 0 & \beta \\ \beta & \alpha-E & \beta & 0 \\ 0 & \beta & \alpha-E & \beta \\ \beta & 0 & \beta & \alpha-E \end{vmatrix} = \begin{vmatrix} \frac{\alpha-E}{\beta} & 1 & 0 & 1 \\ 1 & \frac{\alpha-E}{\beta} & 1 & 0 \\ 0 & 1 & \frac{\alpha-E}{\beta} & 1 \\ 1 & 0 & 1 & \frac{\alpha-E}{\beta} \end{vmatrix} = \begin{vmatrix} -\lambda & 1 & 0 & 1 \\ 1 & -\lambda & 1 & 0 \\ 0 & 1 & -\lambda & 1 \\ 1 & 0 & 1 & -\lambda \end{vmatrix} = 0$$

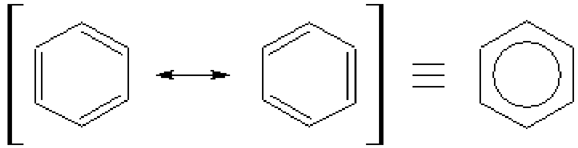
$$-\lambda\begin{vmatrix} -\lambda & 1 & 0 \\ 1 & -\lambda & 1 \\ 0 & 1 & -\lambda \end{vmatrix} - \begin{vmatrix} 1 & 0 & 1 \\ 1 & -\lambda & 1 \\ 0 & 1 & -\lambda \end{vmatrix} - \begin{vmatrix} 1 & 0 & 1 \\ -\lambda & 1 & 0 \\ 1 & -\lambda & 1 \end{vmatrix} = \lambda(\lambda^3-2\lambda)-\lambda^2-\lambda^2 = \lambda^4-4\lambda^2 = \lambda^2(\lambda^2-4) = 0$$

$\lambda = 0$ $\lambda^2 - 4 = 0$ より $\lambda = \pm 2$

$E_1 = \alpha + 2\beta$ $E_2 = E_3 = \alpha$ $E_4 = \alpha - 2\beta$



ベンゼン



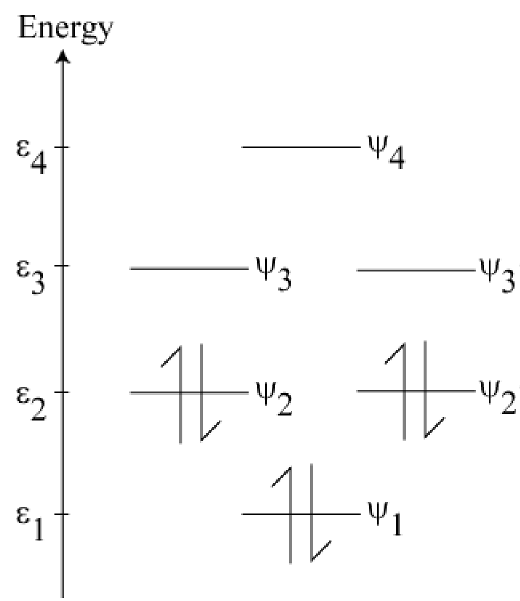
ベンゼンの共鳴

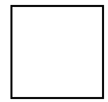
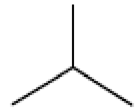
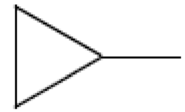
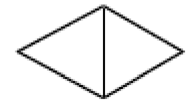
$$\begin{vmatrix} -\lambda & 1 & 0 & 0 & 0 & 1 \\ 1 & -\lambda & 1 & 0 & 0 & 0 \\ 0 & 1 & -\lambda & 1 & 0 & 0 \\ 0 & 0 & 1 & -\lambda & 1 & 0 \\ 0 & 0 & 0 & 1 & -\lambda & 1 \\ 1 & 0 & 0 & 0 & 1 & -\lambda \end{vmatrix} = -\lambda \begin{vmatrix} -\lambda & 1 & 0 & 0 & 0 \\ 1 & -\lambda & 1 & 0 & 0 \\ 0 & 1 & -\lambda & 1 & 0 \\ 0 & 0 & 1 & -\lambda & 1 \\ 0 & 0 & 0 & 1 & -\lambda \end{vmatrix} - \begin{vmatrix} 1 & 0 & 0 & 0 & 1 \\ 1 & -\lambda & 1 & 0 & 0 \\ 0 & 1 & -\lambda & 1 & 0 \\ 0 & 0 & 1 & -\lambda & 1 \\ 0 & 0 & 0 & 1 & -\lambda \end{vmatrix} - \begin{vmatrix} 1 & 0 & 0 & 0 & 1 \\ -\lambda & 1 & 0 & 0 & 0 \\ 1 & -\lambda & 1 & 0 & 0 \\ 0 & 1 & -\lambda & 1 & 0 \\ 0 & 0 & 1 & -\lambda & 1 \end{vmatrix}$$

$= (\lambda - 2)(\lambda - 1)^2(\lambda + 1)^2(\lambda + 2) = 0$　より

$\lambda = -2 \quad -1 \quad 1 \quad 2$

$E_1 = \alpha + 2\beta \quad E_2 = \alpha + \beta \quad E_3 = \alpha + \beta \quad E_4 = \alpha - \beta \quad E_5 = \alpha - \beta \quad E_6 = \alpha - 2\beta$



４×４行列式の小行列への分解

$$\begin{vmatrix} a & x_1 & y_1 & z_1 \\ b & x_2 & y_2 & z_2 \\ c & x_3 & y_3 & z_3 \\ d & x_4 & y_4 & z_4 \end{vmatrix} = a\begin{vmatrix} x_2 & y_2 & z_2 \\ x_3 & y_3 & z_3 \\ x_4 & y_4 & z_4 \end{vmatrix} - b\begin{vmatrix} x_1 & y_1 & z_1 \\ x_3 & y_3 & z_3 \\ x_4 & y_4 & z_4 \end{vmatrix} + c\begin{vmatrix} x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \\ x_4 & y_4 & z_4 \end{vmatrix} - d\begin{vmatrix} x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \\ x_3 & y_3 & z_3 \end{vmatrix}$$

行列式は任意の２行を入れ返るごとに符号が変わる。

$$\begin{vmatrix} a & x_1 & y_1 & z_1 \\ b & x_2 & y_2 & z_2 \\ c & x_3 & y_3 & z_3 \\ d & x_4 & y_4 & z_4 \end{vmatrix} = -\begin{vmatrix} x_1 & a & y_1 & z_1 \\ x_2 & b & y_2 & z_2 \\ x_3 & c & y_3 & z_3 \\ x_4 & d & y_4 & z_4 \end{vmatrix}$$