

Bonding Orbital σ_g $\psi_{\sigma_g} = N_+ (\psi_{1sA} + \psi_{1sB})$

anti-bonding orbital σ_u^* $\psi_{\sigma_u^*} = N_- (\psi_{1sA} - \psi_{1sB})$

Define Coulomb Integral

$$H_{AA} = \int \psi_{1sA}^* \hat{H} \psi_{1sA} d\tau = H_{BB}$$

Resonance integral

$$H_{AB} = \int \psi_{1sA}^* \hat{H} \psi_{1sB} d\tau = H_{BA}$$

$$J = H_{AA} - E_{1s}$$

$$K = H_{AB} - E_{1s} S$$

$$S = \int \psi_{1sA}^* \psi_{1sB} d\tau$$

overlap integral

$$E_{\sigma_g} = E_{1s} + \frac{J+K}{1+S}$$

$$E_{\sigma_u^*} = E_{1s} + \frac{J-K}{1-S}$$

or simpler, forget about J and K.

$$E_{\pm} = \frac{H_{AA} \pm H_{AB}}{1 \pm S}$$



PP. 400 - 402 of Silbey, Alberty...