Answer on Question #55177 - Chemistry - General chemistry

Question:

Normalize the molecular orbital Ψ(1) = ψA(1)+λ ψB(1)in terms of the parameter and the overelap S.

Answer:

$\int \Psi(1)^{*}\Psi(1) = N^2 \int (\Psi_A(1) + \lambda\Psi_B(1))^{*}(\Psi_A(1)+\lambda\Psi_B(1))dv=1$

$N^2 \int (\Psi^{*}_A(1)\Psi_A(1))dv + N^2\lambda^2 \int (\Psi^{*}_B(1)\Psi^{*}_B(1)dv + 2\lambda N^2 \int (\Psi^{*}_B(1)\Psi_A(1))dV = N^2(1+\lambda^2+2S\lambda)$

$$N = \frac{1}{\sqrt{1+\lambda^2+2S\lambda}}$$