

Atoms, Molecules & Reactions, Spring 2006
Quantum Mechanics Homework

1. Generate the following two equations using $\frac{\partial E}{\partial C_1} = 0$ and $\frac{\partial E}{\partial C_2} = 0$

$$C_1 (H_{AA} - E) + C_2 (H_{AB} - ES) = 0 \quad \text{Equation 1}$$

$$C_1 (H_{AB} - ES) + C_2 (H_{AA} - E) = 0 \quad \text{Equation 2}$$

2. Substituting the energy values we obtained in class for H_2^+ in the following equations, obtain a relationship between C_1 and C_2 .

$$C_1 (H_{AA} - E) + C_2 (H_{AB} - ES) = 0 \quad \text{Equation 1}$$

$$C_1 (H_{AB} - ES) + C_2 (H_{AA} - E) = 0 \quad \text{Equation 2}$$

3. Using the relationships you obtained in (2) above and the following facts, calculate the values of C_1 and C_2 .

○ $\psi = C_1 1S_A + C_2 1S_B$

○ The wave function ψ is normalized.

4. Write the complete wave functions you obtained in (3) above. Then draw a rough sketch of these wave functions.