

Atoms, Molecules and Reactions – I
Quantum Mechanics – Week 7 Homework
In addition to the ones on the web site

In class we obtained the following two equations.

$$C_1 [H_{AA} - \langle E \rangle] + C_2 [H_{AB} - S \langle E \rangle] = 0 \quad \text{Equation 1}$$

$$C_1 [H_{AB} - S \langle E \rangle] + C_2 [H_{BB} - \langle E \rangle] = 0 \quad \text{Equation 2}$$

We also calculated two values for the average energy $\langle E \rangle$ as follows.

$$E_1 = \frac{H_{AA} + H_{AB}}{1 + S} \quad \text{and} \quad E_2 = \frac{H_{AA} - H_{AB}}{1 - S}$$

1. Substitute the values of E_1 and E_2 in Equations 1 and 2 and show that $C_1 = C_2$ and $C_1 = -C_2$
2. Then use the fact that ψ for the H_2^+ molecular ion = $C_1 1s_A + C_2 1s_B$ and that $C_1 = \pm C_2$, normalize ψ to obtain values for C_1 and C_2 (these values were given in class).
3. Read the section on correlation diagrams very carefully. We will NOT go over this since we covered it in inorganic chemistry.