

Advanced Chemistry, 2008
Spring Quarter – Week 2 Homework

In class today we evaluated $\langle E \rangle$ for the hydrogen molecular ion using the variation theorem and obtained the following expression.

$$\langle E \rangle = \frac{C_1^2 H_{AA} + 2C_1 C_2 H_{AB} + C_2^2 H_{BB}}{C_1^2 + 2C_1 C_2 S + C_2^2}$$

Use this expression to evaluate the following derivatives. Bring your work to class next week.

$$\frac{\partial \langle E \rangle}{\partial C_1}$$

$$\frac{\partial \langle E \rangle}{\partial C_2}$$