

Name: _____

Please answer all questions, showing all calculations

- Which of the following could be valid wavefunction in the region 0 to infinity? (5 points)
 A) $A \sin^2 kx$ B) $A e^{kx}$ C) $A \sin^2 x e^{-kx}$ D) $A e^{-kx} / \sin x$ E) $A x e^{-x}$
- Which of the following excited state wavefunctions are allowed under the Pauli principle for a He-H molecule where $\psi_1(n)$ and $\psi_2(n)$ refer to spin wavefunctions for the nth electron and $\phi_1(n)$ and $\phi_2(n)$ refer to molecular orbit wavefunctions constructed from 1s and 2s orbitals on the H and He atoms? (15 points)
 - $\phi_1(2) \{ \psi_2(2) - \psi_1(2) \} \{ \phi_1(1) \phi_2(3) - \phi_1(3) \phi_2(1) \}$
 - $\{ \phi_1(1) \phi_1(3) \phi_2(2) - \phi_1(2) \phi_1(3) \phi_2(1) \} \{ \psi_1(1) \psi_2(3) + \psi_1(3) \psi_2(1) \} + \{ \phi_1(1) \phi_1(2) \phi_2(3) - \phi_1(2) \phi_1(3) \phi_2(1) \} \{ \psi_1(1) \psi_2(3) + \psi_1(3) \psi_2(1) \} + \{ \phi_1(2) \phi_1(3) \phi_2(1) \} \{ \psi_1(2) \psi_2(3) - \psi_1(3) \psi_2(1) \}$
 - $\{ \phi_1(1) \phi_1(2) \phi_2(3) - \phi_1(3) \phi_2(1) \phi_1(2) \} \{ \psi_1(1) \psi_2(3) + \psi_1(3) \psi_2(1) \} + \{ \phi_1(2) \phi_2(1) \phi_1(3) - \phi_1(1) \phi_2(2) \phi_1(3) \} \{ \psi_1(1) \psi_2(3) + \psi_1(3) \psi_2(1) \} + \{ \phi_1(3) \phi_1(1) \phi_2(2) - \phi_1(2) \phi_1(1) \phi_2(3) \} \{ \psi_1(3) \psi_2(2) + \psi_1(2) \psi_2(3) \}$
 - $\{ \phi_1(1) \phi_1(2) \phi_2(3) + \phi_1(3) \phi_2(1) \phi_1(2) \} \{ \psi_1(1) \psi_2(3) - \psi_1(3) \psi_2(1) \} + \{ \phi_1(2) \phi_2(1) \phi_1(3) - \phi_1(1) \phi_2(2) \phi_1(3) \} \{ \psi_1(1) \psi_2(3) + \psi_1(3) \psi_2(1) \} + \{ \phi_1(3) \phi_1(1) \phi_2(2) + \phi_1(2) \phi_1(1) \phi_2(3) \} \{ \psi_1(3) \psi_2(2) + \psi_1(2) \psi_2(3) \}$
 - $\phi_1(1) \phi_1(2) \phi_2(3) \psi_1(1) \psi_2(3)$
- What is the bond order for a CF^- molecule? (5 points)
 A) 0 B) 1 C) 1.5 D) 2 E) 2.5
- Describe in your own words the Born-Oppenheimer approximation. (12 points)
- Write the Hückel matrix for the cycloheptatriene carboanion (C_7H_7^- , negative charge on one carbon). Calculate (using Maple) the 7 energy levels (in terms of α and β , usual definitions) which constitute the bonding system and indicate lowest energy transition. (15 points)
- Calculate the absorbance at 550 nm from a solution prepared by mixing 10 ml of 3M CuSO_4 with 10 ml of 2M FeSO_4 and diluted to 100 ml in a 1.0 cm pathlength cell given the molar absorptivity at 550 nm is $\epsilon_{\text{Cu}} = 2300 \text{ M}^{-1} \text{ cm}^{-1}$ and $\epsilon_{\text{Fe}} = 7100 \text{ M}^{-1} \text{ cm}^{-1}$. (10 points)
- Assuming that the dipole moment operator is just $\mu_x = e\mathbf{x}$, calculate the x component of the transition dipole moment from the $n = 1$ to the $n = K$ level in the one-dimensional particle in a box. What transitions will be allowed? (10 points, use Maple to perform required integral.)