**Question 1.** Write down the electronic Hamiltonian in the coordinate representation. You may use atomic units. If you use one-electron and two-electron operators in your answer, please define what they are.

**Question 2.** Explain the difference between the quantum mechanical operator $\hat{H}$ and the algebraic operator $\mathscr{H}$ in one sentence.

**Question 3.** Qualitatively explain what is meant by the equation:

$$|\phi\rangle = \sum_{all\ i} |i\rangle \langle i|\phi\rangle$$

In your explanation, be sure to include the qualitative interpretations of $\langle i|\phi\rangle$, state vector $|\phi\rangle$, state vectors $|i\rangle$, and what we mean by the term "resolution of the identity".

**Question 4.** Qualitatively (i.e., without equations, unless you really prefer it) explain the major steps required to get from the time-independent Schrodinger equation to the Roothaan-Hall equations. Make sure to touch on the following details:

- the Hamiltonian

- the form and composition of the wavefunction

- how the expectation value of the Hamiltonian for this wavefunction $E = \langle \Phi \mid \hat{H} \mid \Phi \rangle$ relates to the Hartree-Fock equations

- how the Hartree-Fock equations relate to the Roothaan-Hall equations

**Question 5.** Beginning from the restricted-determinant form for the 1st Slater-Condon rule:

$$E = 2\sum_i^{N/2}\langle\phi_i|\hat{h}|\phi_i\rangle + \sum_i^{N/2}\sum_j^{N/2} 2\langle\phi_i\phi_j|\hat{g}|\phi_i\phi_j\rangle - \langle\phi_i\phi_j|\hat{g}|\phi_j\phi_i\rangle$$

expand each spatial orbital as a linear combination of atomic orbitals:

$$\langle\phi_i| = \sum_p\langle\chi_p\mid C_{pi}^* \quad |\phi_i\rangle = \sum_q \mid \chi_q\rangle C_{qi} \quad \langle\phi_j| = \sum_r\langle\chi_r\mid C_{rj}^* \quad |\phi_j\rangle = \sum_s \mid \chi_s\rangle C_{sj}$$

and derive the RHF energy expression for molecular orbitals (MOs) approximated by a linear combination of atomic orbital basis functions.

**Question 6.** Suppose you have a basis-set composed of 4 Gaussian basis functions

$$\chi_1(r) \quad \chi_2(r) \quad \chi_3(r) \quad \chi_4(r)$$

Suppose further you perform a *restricted* Hartree-Fock computation (i.e., using the Roothaan-Hall equations) using this basis on a system with 4 electrons and obtain the following molecular orbital coefficients:

$$\mathbf{C} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} \\ C_{21} & C_{22} & C_{23} & C_{24} \\ C_{31} & C_{32} & C_{33} & C_{34} \\ C_{41} & C_{42} & C_{43} & C_{44} \end{bmatrix}$$

where each column above corresponds to the coefficients for one molecular orbital, and the relative energies of each molecular orbital are in increasing order from left to right.
Write down a valid form for the ground-state Slater Determinant wavefunction in terms of the above basis functions $\chi$ and coefficients $C_{ij}$. Make sure to distinguish between different electron's coordinates and include spin functions $\alpha$ and $\beta$ in your answer. You do not need to explicitly expand all permutations of molecular orbital products; you may use the antisymmetrizer operator $\hat{A}$ or use the matrix-like representation for a determinant.