Test-exam (replacement for computational exercise report)

1) Discuss the choices of methods (HF, CCS, CCSD) for computing ground state energies. Your discussion should touch the following topics

- variational principle

- optimization condition

- electron correlation

- size consistency

- computational scaling

2) All calculations you have done are for a closed-shell state. Discuss what this means in terms of eigenvalues of the spin angular momentum operators S2 and Sz. Your discussion should touch the following topics

- allowed values of eigenvalues

- coupling of spin

- spin-symmetry of the excited states

3) [not related to computations] Discuss how time-independent non-degenerate perturbation theory is used in quantum chemistry. Your discussion should touch the following topics

- MP2 (strengths&weaknesses)

- electric molecular properties

The final exam will have tasks of this structure, but since scanning in handwritten papers will not be possible, I will have to add multiple-choice like questions which tests more explicit knowledge of equations and derivations.