

Al-Farabi Kazakh National University
Faculty of chemistry and chemical technology
Department of physical chemistry, catalysis and petrochemistry

Program of the final exam on discipline

91725 Quantum-chemical methods in thermochemistry

6B05301-Chemistry (NIS)

Almaty 2023

The program of the final exam is composed by the lecturer of the Department of Physical Chemistry, Catalysis and Petrochemistry, PhD Supiyeva Zh.A.

Reviewed and recommended at the meeting of the department of physical chemistry, catalysis and petrochemistry

«__» _____ 2023, Protocol № _____

Head of department _____ Ye.A.Aubakirov

Topics for which assignments will be compiled

1. Description of modern quantum chemistry.
2. The atom in computational methods. One electron atom. A multi-electron atom.
3. Semi-empirical methods of electronic structure calculation.
4. Basic functions of Slater and Gaussian types.
5. Approximate methods for solving the Schrödinger equation for multi-electron systems.
6. A molecule in computational methods. Born-Oppenheimer approximation.
7. Approximation of the linear combination of MO atomic orbitals. Roothaan equations.
8. Hartree-Fock method.
9. Basis sets and pseudopotentials.
10. Electronic characteristics.
11. Methods of accounting for electronic correlation. Methods of function theory.
12. Geitler-London, Pauling-Slater method of valence bonds, concepts of hybridization and resonance from the perspective of quantum mechanics.
13. Geitler-London, Pauling-Slater method of valence bonds, concepts of hybridization and resonance from the perspective of quantum mechanics. Homonuclear diatomic molecules, calculation of their MO energy using the variational principle.
14. Designing a task for calculating simple molecules. The problem of choosing the basis of AO. Geometric optimization. Analysis of AO complementation and communication order according to Mulliken.
15. Molecular quantum numbers. MO method-basic rules and tasks. One electron approximation, concept of molecular orbital. Linear combination approximation of MO atomic orbital in the Hartree-Fock method, Roothaan equations and their solution methodology.