Syllabus for PhD entrance test in Computational Sciences

1. **Basic principles and applications of quantum mechanics** – operators, eigen values, eigen functions, hermitian operators, postulates and theorems of quantum mechanics, particle in a 1D/3D box, harmonic oscillator, rigid rotor, hydrogen atom, angular momentum, term symbols and electronic configurations.
2. **Approximate methods in molecular quantum mechanics**- Variational principle and perturbation theory in quantum mechanics and their applications, molecular orbital and valence bond theories, Huckel's MO method, semi-empirical methods, Hartee-Fock method, electron correlation and its treatment- configuration interaction, density functional theory, basis sets in quantum chemistry. Difference between classical and quantum chemical methods
3. **Biomolecular chemistry**– photosystems, porphyrines, metalloenzymes, oxygen transport, electron- transfer reactions, nitrogen fixation, basics of structure and functions of nucleic acids and proteins.
4. **Weak molecular interactions**- Hydrogen bonding, van der Waals interactions and other weak interactions and their presence in biological and chemical structures.
5. **Atomic structure and chemical bonding**- VSEPR theory, hybridization, MO treatment of homonuclear and heteronuclear diatomic molecules
6. **Chemical applications of group theory**- point groups, symmetry elements, vanishing integrals, Jahn-Taller distortions.
7. **Basic principles and applications of spectroscopy**- atomic spectroscopy, rotational (microwave), vibrational (IR), electronic (UV), X-ray, NMR and ESR spectroscopies.
8. **Chemical kinetics** – empirical rate laws, Arrhenius equation, theories of reaction rates, determination of reaction mechanisms, experimental techniques for fast reactions.
9. **Chemical equilibria**- Basic principles, Le-Chatelier principle, factors affecting chemical equilibria, solubility and solubility product.
10. **Chemical thermodynamics**- The First Law of Thermodynamics, Entropy and the Second Law, spontaneity of reactions and thermodynamics, Entropy and the Third Law of Thermodynamics. Helmholtz and Gibbs Energies, Phase Equilibria.