

Quantum Chemistry & Spectroscopy

a lecture course for PhD students, IPC PAS

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List of topics:

1. Experimental basis of quantum mechanics. (Dual nature of light. Diffraction and interference. Compton effect. Photoelectric effect. Blackbody radiation. De Broglie hypothesis. Heisenberg's uncertainty principle.)
2. Schrödinger equation. Concept and interpretation of the wave function.
3. Particle in a box. Tunnelling.
4. Harmonic oscillator – classical and quantum approaches.
5. Rigid quantum rotor.
6. Description of the electron in a hydrogen atom.
7. Orbital and spin angular momentum. Stern-Gerlach experiment. Zeeman effect.
8. Variational principle.
9. Basic properties and interpretation of the wave function of a multi-electronic system. Concepts of atomic and molecular orbitals. Pauli's exclusion principle. Hund's rule.
10. Chemical bonding in diatomic molecules.
11. Basic concepts of group theory. Symmetry and chirality.
12. Probability of spectroscopic transitions. Transition moment and Boltzmann distribution.
13. Microwave spectroscopy of rigid linear molecules.
14. Description of molecular rotations beyond the rigid linear rotor model.
15. Basic concepts of vibrational IR spectroscopy. Anharmonicity and dissociation energy.
16. Basic concepts of Raman spectroscopy.
17. Ro-vibrational spectroscopic transitions.
18. Comparison of classical (dispersive) vs. Fourier-transform spectroscopy.
19. Electronic spectroscopy of atoms.
20. Electronic spectroscopy of molecules. Luminescence. Jablonsky diagram. Photodissociation.
21. Photoelectron spectroscopy.
22. Nuclear magnetic resonance spectroscopy.
23. Electron spin resonance spectroscopy.